ABSORPTION | ADSORPTION | AERATION | AEROBIC | AEROSOL | AGGLOMERATION | ANAEROBIC | ANTIBODY | ATTRITION | AUTOCATALYSIS | AZEOTROPE | BATCH | BILAYERS | BIOCATALYSIS | BIOCHEMICAL ENGINEERING | BIODIESEL | BIOFILM | BIOLOGICAL ENGINEERING | BIOMOLECULE | BIOMOLECULAR ENGINEERING | BIOMEDICAL ENGINEERING | BIOPROCESS | BIOREACTORS | BIOSEPARATION | BIOTECHNOLOGY | BIOTEMPLATING | BUBBLE COLUMNS | BUBBLE | CAPSOMERE | CARBON DIOXIDE | CATALYSIS | CATALYST ACTIVATION | CATALYST DEACTIVATION | CATALYST SELECTIVITY | CATALYST SUPPORT | CELL BIOLOGY | CELL ENGINEERING | CENTRIFUGATION | CFD | CHAOS | CHEMICAL ANALYSIS | CHEMICAL PROCESSES | CHEMICAL REACTORS | CHROMATOGRAPHY | COAGULATION | COLLOID | COMBUSTION | COMPLEXITY | COMPLEX FLUIDS | COMPOSITES | COMPUTATION | COMPUTATIONAL | CHEMISTRY | COMPUTATIONAL FLUID DYNAMICS | CONDENSATION | CONTROL | CONVECTION | CORROSION | CRUSHING | CRYSTALLISATION | DEM | DESALINATION | DESIGN | DESORPTION | DIALYSIS | DIFFUSION | DISCRETE ELEMENT MODELING | DISPERSION | DISSOLUTION | DISTILLATION | DNA | DOWNSTREAM PROCESSING | DROP | DRYING | DUST | DYNAMIC SIMULATION | ECONOMICS | ELASTICITY | ELECTROCHEMISTRY | ELECTROLYSIS | ELECTRONIC MATERIALS | ELECTRO-OSMOSIS | ELECTROPHORESIS | EMULSION | ENERGY | ENTROPY | ENVIRONMENT | ENZYME | EVAPORATION | EXPLOSIONS | EXTRACTION | EXTRUSION | FERMENTATION | FILMS | FILTRATION | FLOTATION | FOOD | FLUID MECHANICS | FLUIDIZATION | FOAM FOOD PROCESSING | FORMULATION | FOULING | FRACTALS | FUEL | GASES | GELS | GRANULATION | GRANULAR MATERIALS | GREENHOUSE GAS | HEAT CONDUCTION | HEAT TRANSFER | HOMOGENIZATION | HYDRATE | HYDRODYNAMICS | IMAGING | INSTRUMENTATION | INTERFACE | INTERFACIAL TENSION | INTERFACIAL RHEOLOGY | ION EXCHANGE | ISOTHERMAL | KINETICS | LAMINAR FLOW | LEACHING | MASS TRANSFER | MATERIALS | MATHEMATICAL MODELLING | MEMBRANES | METABOLISM | MICROELECTRONICS | MICROREACTOR | MICROFLUIDIC | MICROSTRUCTURE | MIXING | MODEL REDUCTION | MOLDING | MOULDING | MOLECULAR BIOLOGY | MOLECULAR ENGINEERING | MOMENTUM TRANSFER | MONOCLONAL ANTIBODY | MORPHOLOGY | MOVING BED | MULTIPHASE FLOW | MULTIPHASE REACTIONS | MULTIPHASE REACTORS | MULTISCALE | NANOMATERIALS | NANOSTRUCTURE

2017

AIChE® ANNUAL MEETING

CONFERENCE PROGRAM | OCTOBER 29 - NOVEMBER 3, 2017 | MINNEAPOLIS, MN

ANALYSIS | OPTIMISATION | PACKED BED | PARAMETER IDENTIFICATION | PARTICLE | PARTICLE FORMATION | PARTICLE PROCESSING | PARTICULATE PROCESSES | PEPTIDE | PETROLEUM | PHARMACEUTICALS | PHASE CHANGE | PHASE EQUILIBRIA | PHOTOCHEMISTRY | PIV | PNEUMATIC CONVEYING | POLLUTION | POLYMERS | POLYMER PROCESSING | POLYMERISATION | POPULATION BALANCE POROUS MEDIA | POWDER TECHNOLOGY | POWDERS | PRECIPITATION | PROCESS INTENSIFICATION | PRODUCT DESIGN | PROCESS SYSTEMS | PRODUCT PROCESSING | PROTEIN | RADIATION | REACTION ENGINEERING | REMEDIATION | RENEWABLE ENERGY | RHEOLOGY | SAFETY | SCALE-UP | SEDIMENTATION | SELECTIVITY | SEPARATIONS | SEQUESTRATION | SIMULATION | SINTERING | SLURRIES | SOFT SOLIDS | SOLAR ENERGY | SOLID MECHANICS | SOLUTIONS | STABILITY | STATE EQUATION | STATIC MIXER | STATISTICAL THERMODYNAMICS | SUPERCRITICAL FLUID | SUSTAINABILITY | SURFACTANT | SUSPENSION | SYNTHETIC BIOLOGY | SYSTEMS ENGINEERING | THEORY OF LIQUIDS | THERMODYNAMICS PROCESS | TISSUE ENGINEERING | TOMOGRAPHY | TRANSIENT RESPONSE | TRANSPORT PROCESSES | TURBULENCE | UNIT OPERATIONS | VACCINE | VAPORIZATION | VIRUS-LIKE PARTICLE | VISCOELASTICITY | VISUALISATION | VOIDAGE | WASTE TREATMENT | WATER | WIND ENERGY | ZEOLITES | ABSORPTION | ADSORPTION | AERATION | AEROBIC | AEROSOL | AGGLOMERATION | ANAEROBIC | ANTIBODY | ATTRITION | AUTOCATALYSIS | AZEOTROPE | BATCH | BILAYERS | BIOCATALYSIS | BIOCHEMICAL ENGINEERING | BIODIESEL | BIOFILM | BIOLOGICAL ENGINEERING | BIOMOLECULE | BIOMOLECULAR ENGINEERING | BIOMEDICAL ENGINEERING | BIOPROCESS | BIOREACTORS | BIOSEPARATION | BIOTECHNOLOGY | BIOTEMPLATING | BUBBLE COLUMNS | BUBBLE | CAPSOMERE | CARBON DIOXIDE | CATALYSIS | CATALYST ACTIVATION | CATALYST DEACTIVATION | CATALYST SELECTIVITY | CATALYST SUPPORT | CELL BIOLOGY | CELL ENGINEERING | CENTRIFUGATION | CFD | CHAOS | CHEMICAL ANALYSIS | CHEMICAL PROCESSES | CHEMICAL REACTORS | CHROMATOGRAPHY | COAGULATION | COLLOID | COMBUSTION | COMPLEXITY | COMPLEX FLUIDS | COMPOSITES

17AIChE

Annual Meeting, Minneapolis, MN

2017 ANNUAL MEETING CONTENTS

TABLE OF CONTENTS

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

SOCIETAL IMPACT | PROFESSIONAL DEVELOPMENT | NEXT GEN | EDUCATION | CUTTING EDGE | COMMUNITY OF CHENECTIONS

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.

2017 ANNUAL MEETING WELCOME

Dear Colleagues:

On behalf of the Board of Directors, I am happy to welcome you to Minneapolis and the 2017 AIChE® Annual Meeting.

This meeting caps off a dynamic year for AIChE, highlighted by the launch of the DOE-funded Rapid Advancement in Process Intensification Deployment (RAPID) Manufacturing Institute and increasing activities in bioengineering and energy. Also, the AIChE Foundation, led by Eduardo Glandt, continues its good works, with expanded initiatives in safety training, inclusiveness, education, and innovation. Our Annual Meeting program reflects this progress, with new topical conferences dedicated to *Next-Gen Manufacturing*, *Microbiomes and Microbial Communities*, *Thermal Deconstruction of Biomass*, and an *NH_3 Energy*+ conference devoted to ammonia's role in the hydrogen economy.

Other topical conferences return with expanded contents, including *Process Intensification and Modular Chemical Processing*; *Chemical Engineers in Medicine*; and the *Food-Energy-Water Nexus*. Our meeting also incorporates the International Congress on Energy (ICE), featuring a solar power symposium, as well as conferences on nanotechnology, nanomaterials, fossil energy R&D, green process engineering, sensors, and the annual meeting of the AES Electrophoresis Society.

The Annual Meeting also showcases some of our profession's thought leaders:

- Tuesday morning, José Roberto Nunhez of the University of Campinas, Brazil, discusses computational fluid dynamics in mixing at the *IACChE James Y. Oldshue Award Lecture*.
- Next, Tuesday's *Andreas Acrivos Professional Progress Award Lecture* will be presented by Christopher Jones of Georgia Tech, who will describe new techniques for removing CO_2 from dilute gas streams.
- Tuesday evening, the Society for Biological Engineering's *James E. Bailey Award* lecture will be presented by Antonios Mikos of Rice University, whose presentation focuses on biomaterials for tissue engineering.
- Wednesday's *John M. Prausnitz AIChE Institute Lecture* will be delivered by G. V. Rex Reklaitis of Purdue University, who will discuss the role that process systems engineering plays in pharmaceuticals. This lectureship is endowed by the AIChE Foundation.

Special events on Sunday include a *Meet the Faculty Candidates Poster Session*, a *Public Policy Town Hall* hosted by AIChE's Public Affairs and Information Committee, and the annual *Honors Ceremony*. A highlight of Monday's program is a *Meet the Executives* panel entitled "Innovating for a Sustainable Future," featuring perspectives from companies including BASF, Cargill, Chevron, Dow Chemical, and Owens Corning.

The breadth of our technical specializations is matched by the diversity of the people who pursue those interests. This meeting includes a new plenary – *Diversity and Inclusion: Starting and Thriving in the Workplace* on Tuesday morning, as well as forums dedicated to advancing the inclusion and professional prospects of women, underrepresented minorities, LGBTQ members, and disabled engineers.

You may notice that a large contingent of ChE students is in town for our Annual Student Conference (Oct. 27–30). You'll get to meet many of these young engineers at Sunday's 19th Annual Chem-E-Car Competition® and Monday's Student Poster Session.

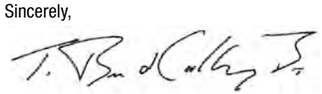
You can also enrich your conference experience by spending time with our exhibitors during the Monday and Tuesday morning coffee breaks, attending poster sessions, and mingling at our nightly receptions.

To keep track of it all, download AIChE's Annual Meeting app and maintain a schedule on your mobile device. And, to ensure a safe and enjoyable time, please read the safety information included in your program book and posted by your hotel.

Finally, the leadership of AIChE extends its gratitude to the meeting's sponsors for their critical support. Thank you, too, to the legions of presenters and authors for sharing their knowledge, and to AIChE's indispensible network of volunteers for making this meeting possible.

I hope that you have a wonderful and productive time in Minneapolis.

Sincerely,



T. Bond Calloway, Jr.
2017 AIChE President

MEETING PROGRAM & GENERAL ARRANGEMENTS CHAIRS

MEETING PROGRAM CHAIR

Sipho C. Ndlela, PhD
Senior Process Engineer
Owens Corning

MEETING PROGRAM CO-CHAIR

David Reeder, PhD
Senior Project Manager
Starches & Sweeteners North America
Cargill

GENERAL ARRANGEMENTS CHAIR

Cristina U. Thomas, PhD
Senior Technical Leader
3M Corporate R&D Services Center

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statgraphics 18

WILEY

BRONZE

ACS Combinatorial Science

ACS SyntheticBiology

AIP Physics of Fluids

apc
Your Process Design & Innovation Partner

BC Bioconjugate Chemistry

I&EC research
Industrial & Engineering Chemistry Research

Journal of chemical & engineering data

SSPC
Innovation Through Collaboration

2017 ANNUAL MEETING EXHIBITORS

- Activated Research Company
- Alliant Insurance Services
- ANSYS *
- AON Affinity
- B&P Littleford
- Biolin Scientific
- Bruker Corporation
- CACHE Corporation
- Cambridge University Press
- Cargill
- CDS Analytical
- Chemstations *
- Clean Energy Smart Manufacturing Innovation Institute (CESMII)
- COSMOlogic GmbH & Co. KG
- CRC Press
- De Gruyter
- DIPPR
- Equilibar, LLC
- Hanwha TOTAL Petrochemical
- Hiden Isochema
- Idaho National Lab
- Imperial College London
- Indian Oil Corporation Limited *
- INFICON
- IntraMicron, Inc.
- JSOL Corporation
- Malvern Instruments
- Michigan State University Properties, Reactions and Separations Facility
- MilliporeSigma
- Molecular Knowledge Systems
- National Energy Technology Laboratory
- National Renewable Energy Laboratory
- Oxford Lasers
- Parr Instrument Company
- Process Systems Enterprise *
- Riogen
- Royal Society of Chemistry
- Savannah River National Laboratory
- **Schneider Electric Software †**
- Siemens PLM Software *
- **Statgraphics Technologies, Inc. †**
- Surface Measurement Systems
- TA Instruments
- TechnipFMC
- **Teledyne Isco †**
- Tridiagonal Solutions Inc.
- VisiMix
- Wiley
- Workrite Uniform Company

* Sponsored Technology Workshop Scheduled

† Featured Exhibitor

Process Intensification Section of Exhibit

Exhibitors as of September 29, 2017.

A NOTE ON PHOTOGRAPHY AND VIDEOGRAPHY FROM THE MEETING ORGANIZERS

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

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

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

Thank you.

SAFETY TIPS

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

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

AIChE ANNUAL MEETING REGISTRATION

EXHIBIT HALL B, MINNEAPOLIS CONVENTION CENTER

Saturday, October 28	Noon – 5:00 PM
Sunday, October 29	8:00 AM – 8:00 PM
Monday, October 30	7:00 AM – 5:30 PM
Tuesday, October 31	7:00 AM – 5:30 PM
Wednesday, November 1	7:00 AM – 5:30 PM
Thursday, November 2	7:00 AM – 5:30 PM
Friday, November 3	8:00 AM – 10:00 AM

AIChE ANNUAL MEETING EXHIBIT

EXHIBIT HALL B, MINNEAPOLIS CONVENTION CENTER

Sunday, October 29	7:00 PM – 8:00 PM
Monday, October 30	9:30 AM – 6:00 PM
Tuesday, October 31	9:30 AM – 6:00 PM

AIChE ANNUAL MEETING COFFEE BREAKS & REFRESHMENTS

EXHIBIT HALL B, MINNEAPOLIS CONVENTION CENTER

Monday, October 30	10:30 AM – 11:00 AM
Tuesday, October 31	10:30 AM – 11:00 AM

REFRESHMENTS WILL ALSO BE AVAILABLE AT THE FOLLOWING EVENTS:

AIChE Annual Meeting Opening Reception
Exhibit Hall B, Minneapolis Convention Center
Sunday, October 29 — 7:00 PM – 8:00 PM

AIChE Annual Meeting Poster Receptions
Exhibit Hall B, Minneapolis Convention Center
Monday, October 30 - Wednesday, November 1 — 3:15 PM – 4:45 PM

2017 Andreas Acrivos Award for Professional Progress in Chemical Engineering Lecture
Ballroom B, Minneapolis Convention Center
Tuesday, October 31 — 11:15 AM – 12:15 PM

John M. Prausnitz AIChE Institute Lecture
Ballroom B, Minneapolis Convention Center
Wednesday, November 1 — 11:15 AM – 12:15 PM

BEVERAGE/SNACK STANDS

OUTSIDE OF EXHIBIT HALL B, MINNEAPOLIS CONVENTION CENTER

Sunday, October 29 - Thursday, November 2
Open 7:00 AM - 5:00 PM (Breakfast served until 10:30 AM)
Mill City Food Court Breakfast Express Café Breakfast Sandwiches, Oatmeal, and More
Mill City Grill American Cuisine, including Hamburgers, Hot Dogs, Pizza, and Fries

Sunday, October 29 - Wednesday, November 1
Open 10:30 AM - 2:30 PM
Mill City Food Court Burrito Bar Made-to-order Burritos and Burrito Bowls
Mill City Food Court Sub Express Made-to-order Sandwiches and Subs

Grab your lunch and go. Plenty of seating available in the Exhibit Hall!

WIC FAMILY ACCOMMODATIONS ROOM

DIRECTORS ROW 4, HILTON MINNEAPOLIS

Sunday, October 29 – Friday, November 3	6:30 AM – 6:00 PM*

**Ending at 5:00 PM on Friday, November 3*

Working at Cargill is an opportunity to *thrive*—

a place to develop your career to the fullest while engaging in meaningful work that makes a positive impact around the globe.

Since our founding in 1865, Cargill has grown continuously. And so has our commitment to feeding the world in a responsible way, reducing environmental impact and improving the communities where we live and work. We have:

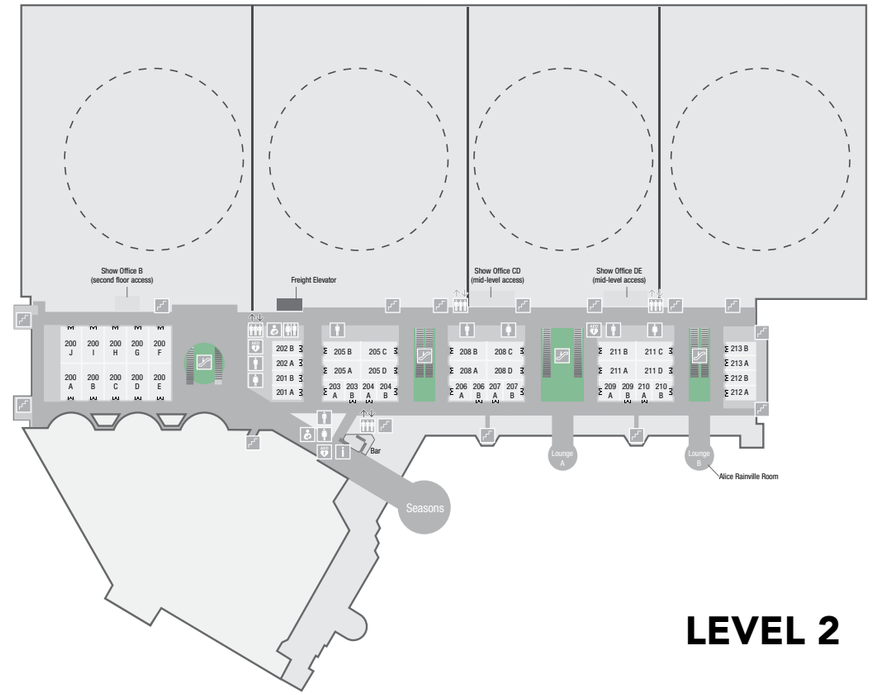
- Approximately 142,000 employees in 67 countries, with more than half in developing countries
- 69 unique business units providing food, agriculture, financial and industrial products and services
- Customers in 125+ countries with annual sales/revenues more than $136 billion
- Nearly limitless opportunities for you to contribute and make a positive difference

At Cargill you will be proud to work for a company with a strong history of ethics and a purpose of nourishing people. We offer a diverse, supportive environment where you will grow personally and professionally as you learn from some of the most talented people in your field.

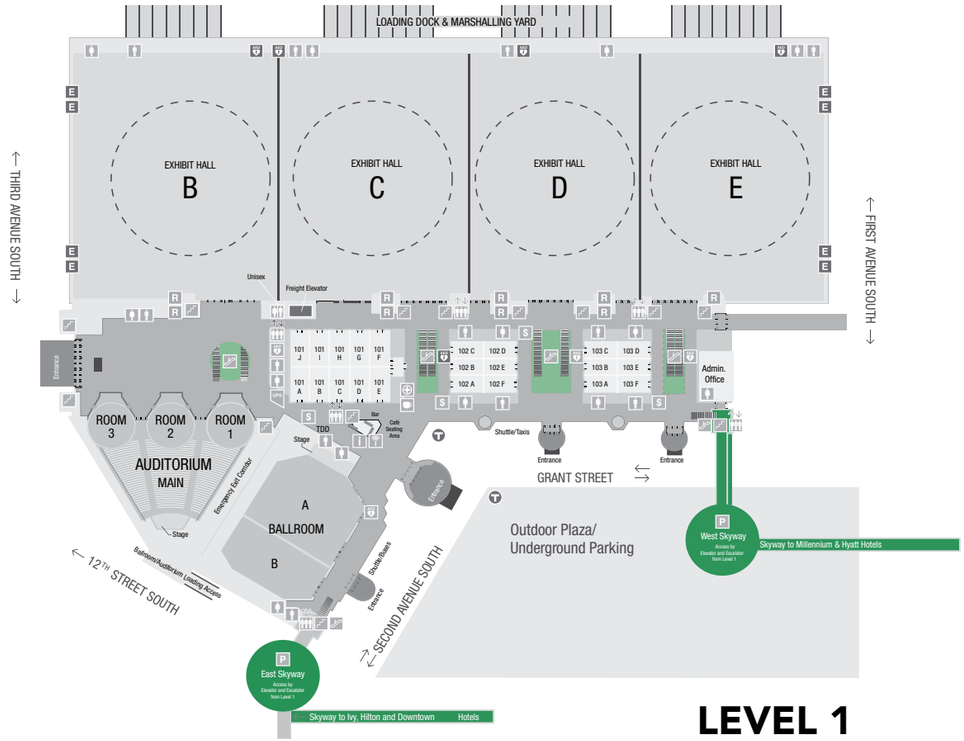
With innovation, creativity, teamwork and diversity as our strengths, we're transforming entire markets – and people's lives. We can have the same incredible impact on your career. And, with literally dozens of business areas where you can apply your talents, a career with Cargill can take you to places you might never have imagined.

Learn more and apply online at www.cargill.com/careers.

Cargill®

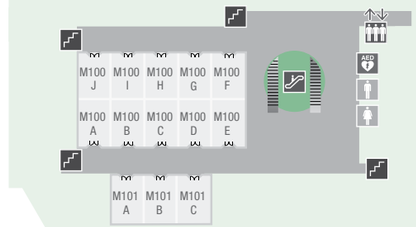


LEVEL 2

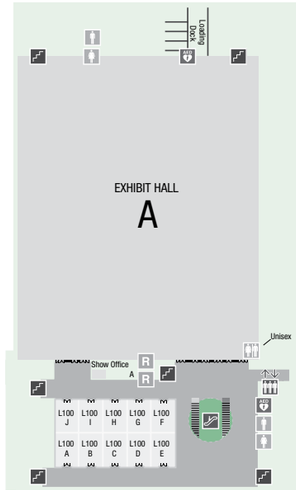


LEVEL 1

MINNEAPOLIS CONVENTION CENTER



MEZZANINE



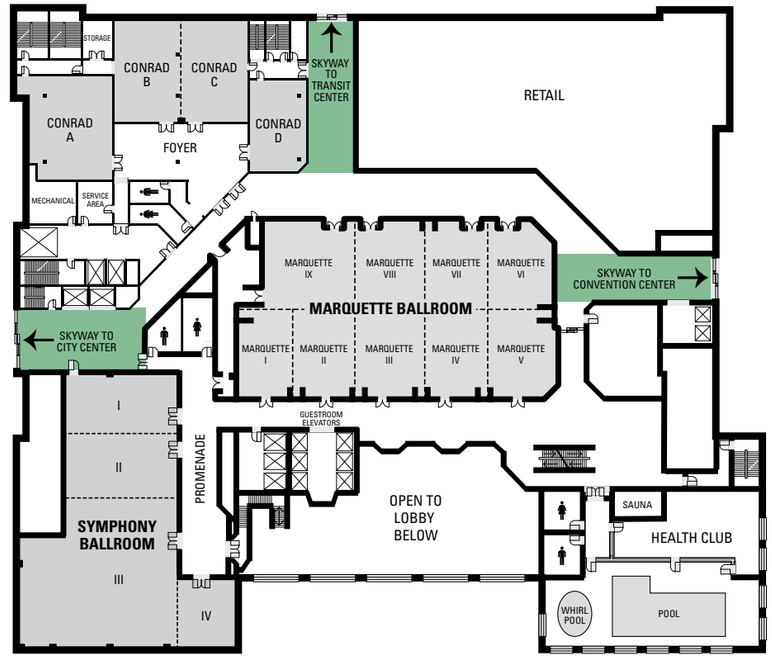
LOWER LEVEL

LEGEND

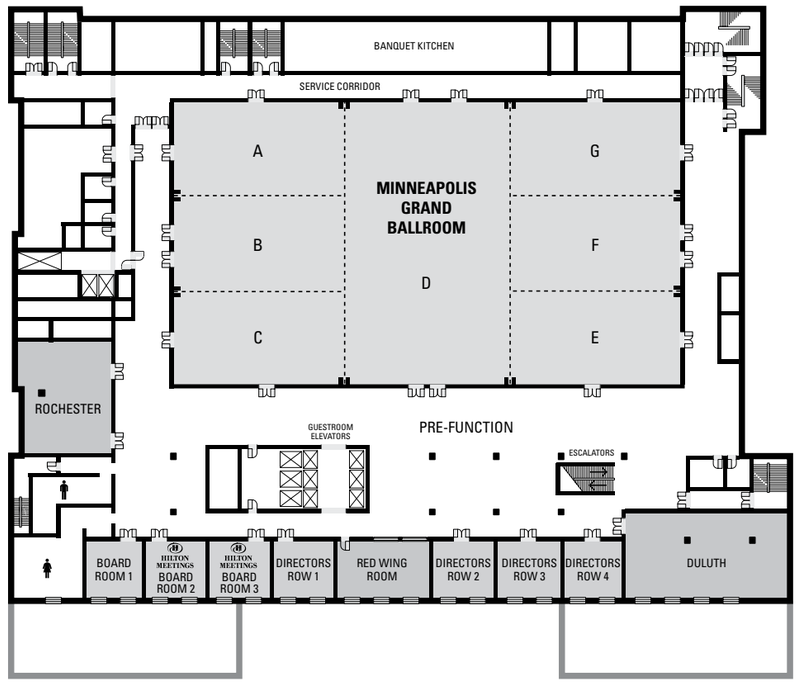
- Restrooms
- Escalators (All Levels)
- Elevators (All Levels)
- Stairs (Levels 1 & 2)
- Emergency Stairs
- Automated External Defibrillator
- Refreshments

MINNEAPOLIS CONVENTION CENTER

SECOND FLOOR



THIRD FLOOR



Note that *The Gallery* is found on the Lobby Level of the Hilton Minneapolis and is accessible from the lobby.

HILTON MINNEAPOLIS

2017 ANNUAL MEETING PROGRAM GRID KEY

The full technical program of the 2017 AIChE® Annual Meeting is comprised of original programming from 22 of AIChE's Divisions and Forums, 10+ topical conferences, and a number of committees. Over 5,500 presentations will take place throughout the week of the Annual Meeting.

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

See below for a list of the subject areas covered at the 2017 AIChE Annual Meeting.

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

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

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

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

05 - Management Division
- 05A - Professional Development

06 - North American Mixing Forum

07 - Transport and Energy Processes

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

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

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

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

2017 ANNUAL MEETING PROGRAM GRID KEY

14 - Nuclear Engineering Division
15 - Food, Pharmaceutical & Bioengineering Division
- 15A - Food
- 15B - Pharmaceuticals
- 15C - Bioengineering
- 15D - Engineering Fundamentals in Life Science

16 - Fuels and Petrochemicals Division
- 16D - Alternate Fuels and New Technology

17 - Forest and Plant Bioproducts Division
18 - Liaison Functions
- 18A - Miscellaneous
- 18B - Public Affairs and Information Committee
- 18C - Young Professionals Committee (YPC)
- 18D - Publication Committee
- 18E - Awards Committee
- 18G - Societal Impact Operating Council (SIOC)
- 18I - Minority Affairs Committee (MAC)
- 18J - Research and New Technology Committee
- 18L - International Committee
- 18M - Women's Initiatives Committee (WIC)
- 18N - Assembly of Fellows

20 - Catalysis and Reaction Engineering Division
21 - Computational Molecular Science & Engineering Forum
22 - Nanoscale Science and Engineering Forum
- 22A - Carbon Nanomaterials
- 22B - Bionanotechnology

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

24 - Chemical Engineering & the Law Forum
25 - Upstream Engineering and Flow Assurance Forum
26 - Pharmaceutical Discovery, Development & Manufacturing Forum

T1 - Meet the Faculty Candidate Poster Session – Sponsored by the Education Division
T3 - 2017 Annual Meeting of the AES Electrophoresis Society
T4 - 2017 International Congress on Energy (ICE)
- T4A - Biorefinery Technologies for Forest Based Lignocellulosic Biomass
- T4B - Symposium on Solar Power & Chemical Systems in Honor of Prof. Edward A. Fletcher
- T4C - Hydrogen Production and Storage
- T4E - Alternative Energy & Enabling Technologies
- T4F - BioFuels
- T4G - Fossil Fuels & CCS
- T4H - International Congress on Energy (ICE) 2017

T5 - Nanomaterials for Applications in Energy & Biology
T6 - Next-Gen Manufacturing
T7 - The Food-Energy-Water Nexus
T8 - Process Intensification & Modular Chemical Processing
T9 - Sensors
TA - Microbiomes and Microbial Communities
TB - Thermal Deconstruction of Biomass
TC - Environmental Aspects, Applications, and Implications of Nanomaterials and Nanotechnology
TD - NH_3 Energy$^+$ - Enabling Optimized, Sustainable Energy and Agriculture
TE - Advances in Fossil Energy R&D
TF - Chemical Engineers in Medicine
TG - Innovations of Green Process Engineering for Sustainable Energy and Environment

Property Key
Hilton = Hilton Minneapolis
MCC = Minneapolis Convention Center

01A - Thermodynamics and Transport Properties

Day	Time	Session #	Session Title	Property	Room
Monday	8:00 AM	70	Faculty Candidates in CoMSEF I: Biomolecules, Soft Materials, and Algorithms*	MCC	L100H
Monday	8:00 AM	83	Modeling of Interfacial Systems*	MCC	M100A
Monday	8:00 AM	84	Molecular Simulation of Surface, Interface and Confinement Effects - In Honor of Keith Gubbins' 80th Birthday I (Invited Talks)	MCC	L100I
Monday	12:30 PM	140	Effects of Confinement on Molecular Properties	MCC	L100J
Monday	12:30 PM	147	Fundamental, Theory, and Model Development - In Honor of Keith Gubbins' 80th Birthday II (Invited Talks)*	MCC	L100H
Monday	12:30 PM	152	In Honor of Stuart W. Churchill I (Invited Talks)*	MCC	101E
Monday	12:30 PM	163	Molecular Simulation and Modeling of Complex Molecules	MCC	L100I
Monday	12:30 PM	176	Solve this! Fundamental Approach to Problem Solving in Industrial Processes I (Invited Talks)*	MCC	101I
Monday	3:15 PM	204	Poster Session: Thermodynamics and Transport Properties (Area 1A)	MCC	Exhibit Hall B
Monday	3:15 PM	213	ChE Potpourri: Beer and Thermodynamics*	MCC	205D
Monday	3:15 PM	218	Faculty Candidates in CoMSEF II: Energy, Catalysis, and Interfaces*	MCC	L100H
Monday	3:15 PM	228	In Honor of Stuart W. Churchill II (Invited Talks)*	MCC	101E
Monday	3:15 PM	240	Solve this! Fundamental Approach to Problem Solving in Industrial Processes II (Invited Talks)*	MCC	101I
Tuesday	8:00 AM	286	Gas Hydrates Science and Engineering	MCC	L100I
Tuesday	8:00 AM	305	New Frontiers of Molecular Thermodynamics (Invited Talks)	MCC	L100J
Tuesday	12:30 PM	365	In Honor of Marco Satyro I (Invited Talks)	MCC	L100I
Tuesday	12:30 PM	392	Thermophysical Properties and Phase Behavior I	MCC	L100J
Tuesday	3:15 PM	431	In Honor of Marco Satyro II (Invited Talks)	MCC	L100I
Tuesday	3:15 PM	453	Thermophysical Properties and Phase Behavior II: Electrolytes and Ionic Liquids	MCC	L100J
Wednesday	8:00 AM	511	Thermodynamics of Biomolecular Folding and Assembly	MCC	L100I
Wednesday	8:00 AM	512	Thermophysical Properties and Phase Behavior III: Complex Molecules and Mixtures	MCC	L100J
Wednesday	12:30 PM	574	Thermophysical Properties and Phase Behavior IV: Theory and Equations of State	MCC	L100J
Wednesday	12:30 PM	575	Thermophysical Properties of Biological Systems	MCC	L100I
Wednesday	3:15 PM	613	Modeling of Lipid Membranes and Membrane Proteins	MCC	L100I
Wednesday	3:15 PM	614	Molecular Simulation of Adsorption I - In Honor of Keith Gubbins' 80th Birthday III (Invited Talks)*	MCC	M100E
Thursday	8:00 AM	683	Nucleation and Growth*	MCC	M100J
Thursday	8:00 AM	685	Recent Advances in Molecular Simulation III: Free Energy and Phase Equilibrium	MCC	L100J
Thursday	8:00 AM	688	Thermodynamics at the Nanoscale	MCC	L100I

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01A - Thermodynamics and Transport Properties (continued)

Thursday	12:30 PM	704	Computational Studies of Self-Assembly	MCC	L100I
Thursday	12:30 PM	708	Development of Intermolecular Potential Models	MCC	L100J
Thursday	3:15 PM	754	Interfacial Phenomena in Ionic Liquids*	MCC	M100B

01C - Interfacial Phenomena

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	27	In Honor of Dennis Prieve's Retirement I (Invited Talks)	MCC	101A
Monday	8:00 AM	83	Modeling of Interfacial Systems	MCC	M100A
Monday	8:00 AM	93	Solid-Liquid Interfaces	MCC	M100B
Monday	12:30 PM	150	In Honor of Dennis Prieve's Retirement II (Invited Talks)	MCC	M100B
Monday	12:30 PM	176	Solve this! Fundamental Approach to Problem Solving in Industrial Processes I (Invited Talks)*	MCC	101I
Monday	3:15 PM	195	Poster Session: Interfacial Phenomena (Area 1C)	MCC	Exhibit Hall B
Monday	3:15 PM	240	Solve this! Fundamental Approach to Problem Solving in Industrial Processes II (Invited Talks)*	MCC	101I
Tuesday	8:00 AM	261	Area Plenary: Interfacial Phenomena (Invited Talks)	MCC	M100B
Tuesday	12:30 PM	360	Fundamentals of Interfacial Phenomena I	MCC	M100B
Tuesday	3:15 PM	409	Anisotropic Particles: Synthesis, Characterization, Modeling, Assembly, and Applications	MCC	M100A
Tuesday	3:15 PM	425	Fundamentals of Interfacial Phenomena II	MCC	M100B
Wednesday	8:00 AM	464	Biomolecules at Interfaces I	MCC	M100B
Wednesday	8:00 AM	488	Interfacial Transport Phenomena	MCC	M100A
Wednesday	12:30 PM	527	Biomolecules at Interfaces II	MCC	M100B
Wednesday	12:30 PM	543	Dynamic Processes at Interfaces	MCC	M100A
Wednesday	3:15 PM	588	Active Colloidal Systems	MCC	M100A
Wednesday	3:15 PM	629	Self-Assembly in Solution	MCC	M100B
Thursday	8:00 AM	654	Colloidal Dispersions	MCC	M100A
Thursday	8:00 AM	669	Interfacial Aspects of Oil/Gas Recovery and Remediation	MCC	M100B
Thursday	12:30 PM	713	Emulsions and Foams	MCC	M100A
Thursday	12:30 PM	718	Interfacial Phenomena in Electrochemical Systems	MCC	M100B
Thursday	3:15 PM	749	Directed and Self Assembly of Colloids	MCC	M100A
Thursday	3:15 PM	754	Interfacial Phenomena in Ionic Liquids	MCC	M100B

01C - Interfacial Phenomena

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	27	In Honor of Dennis Prieve's Retirement I (Invited Talks)	MCC	101A
Monday	8:00 AM	83	Modeling of Interfacial Systems	MCC	M100A
Monday	8:00 AM	93	Solid-Liquid Interfaces	MCC	M100B
Monday	12:30 PM	150	In Honor of Dennis Prieve's Retirement II (Invited Talks)	MCC	M100B

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2017 TECHNICAL PROGRAM GRID

01C - Interfacial Phenomena (continued)					
Monday	12:30 PM	176	Solve this! Fundamental Approach to Problem Solving in Industrial Processes I (Invited Talks)*	MCC	101I
Monday	3:15 PM	195	Poster Session: Interfacial Phenomena (Area 1C)	MCC	Exhibit Hall B
Monday	3:15 PM	240	Solve this! Fundamental Approach to Problem Solving in Industrial Processes II (Invited Talks)*	MCC	101I
Tuesday	8:00 AM	261	Area Plenary: Interfacial Phenomena (Invited Talks)	MCC	M100B
Tuesday	12:30 PM	360	Fundamentals of Interfacial Phenomena I	MCC	M100B
Tuesday	3:15 PM	409	Anisotropic Particles: Synthesis, Characterization, Modeling, Assembly, and Applications	MCC	M100A
Tuesday	3:15 PM	425	Fundamentals of Interfacial Phenomena II	MCC	M100B
Wednesday	8:00 AM	464	Biomolecules at Interfaces I	MCC	M100B
Wednesday	8:00 AM	488	Interfacial Transport Phenomena	MCC	M100A
Wednesday	12:30 PM	527	Biomolecules at Interfaces II	MCC	M100B
Wednesday	12:30 PM	543	Dynamic Processes at Interfaces	MCC	M100A
Wednesday	3:15 PM	588	Active Colloidal Systems	MCC	M100A
Wednesday	3:15 PM	629	Self-Assembly in Solution	MCC	M100B
Thursday	8:00 AM	654	Colloidal Dispersions	MCC	M100A
Thursday	8:00 AM	669	Interfacial Aspects of Oil/Gas Recovery and Remediation	MCC	M100B
Thursday	12:30 PM	713	Emulsions and Foams	MCC	M100A
Thursday	12:30 PM	718	Interfacial Phenomena in Electrochemical Systems	MCC	M100B
Thursday	3:15 PM	749	Directed and Self Assembly of Colloids	MCC	M100A
Thursday	3:15 PM	754	Interfacial Phenomena in Ionic Liquids	MCC	M100B

01D - Transport Processes					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Monday	12:30 PM	152	In Honor of Stuart W. Churchill I (Invited Talks)*	MCC	101E
Monday	12:30 PM	176	Solve this! Fundamental Approach to Problem Solving in Industrial Processes I (Invited Talks)*	MCC	101I
Monday	3:15 PM	228	In Honor of Stuart W. Churchill II (Invited Talks)*	MCC	101E
Monday	3:15 PM	240	Solve this! Fundamental Approach to Problem Solving in Industrial Processes II (Invited Talks)*	MCC	101I
Tuesday	8:00 AM	257	Advances in Process Intensification: Enhanced Mass Transfer*	MCC	101E
Tuesday	12:30 PM	358	Fundamental Research in Transport Processes	MCC	M100D
Tuesday	3:15 PM	435	Mathematical Modeling of Transport Processes	MCC	M100D

01E - Electrochemical Fundamentals					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Monday	8:00 AM	66	Electrocatalysis and Photoelectrocatalysis I: CO2Reduction*	MCC	L100D
Monday	12:30 PM	141	Electrocatalysis and Photoelectrocatalysis II: HER/HOR*	MCC	L100D
Monday	12:30 PM	176	Solve this! Fundamental Approach to Problem Solving in Industrial Processes I (Invited Talks)*	MCC	101I

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01E - Electrochemical Fundamentals (continued)					
Monday	3:15 PM	216	Electrocatalysis and Photoelectrocatalysis III: Computational Methods*	MCC	L100D
Monday	3:15 PM	240	Solve this! Fundamental Approach to Problem Solving in Industrial Processes II (Invited Talks)*	MCC	101I
Tuesday	8:00 AM	282	Electrocatalysis and Photoelectrocatalysis IV: ORR/OER*	MCC	L100D
Tuesday	8:00 AM	320	Tutorial Session on Electrochemical Methods, Systems and Applications (Invited Talks)	MCC	M100C
Tuesday	12:30 PM	351	Electrocatalysis and Photoelectrocatalysis V: Electrolysis and Solar Fuels*	MCC	L100D
Tuesday	12:30 PM	352	Electrochemical Fundamentals: Faculty Candidate Session	MCC	M100C
Tuesday	3:15 PM	422	Electrocatalysis and Photoelectrocatalysis VI: Fuel Oxidation and Chemical Transformations*	MCC	L100D
Tuesday	3:15 PM	433	Invited Symposium: Nature-Inspired Electrochemical Systems	MCC	M100C
Wednesday	8:00 AM	482	Fundamentals of Electrode Processes I	MCC	M100C
Wednesday	12:30 PM	554	Fundamentals of Electrode Processes II	MCC	M100C
Wednesday	3:15 PM	603	Fundamentals of Electrode Processes III	MCC	M100C
Thursday	8:00 AM	670	Lithium and Beyond: Fundamental Advances in High Performance Batteries I	MCC	M100C
Thursday	12:30 PM	718	Interfacial Phenomena in Electrochemical Systems*	MCC	M100B
Thursday	12:30 PM	719	Lithium and Beyond: Fundamental Advances in High Performance Batteries II	MCC	M100C

01F - High Pressure					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Monday	8:00 AM	80	Materials Synthesis and Processing with Compressed or Supercritical Fluids	MCC	M100C
Monday	8:00 AM	90	Reactions in Near-Critical and Supercritical Fluids*	MCC	L100B
Monday	12:30 PM	179	Thermodynamic and Transport Properties Under Pressure	MCC	M100C
Monday	3:15 PM	225	High Pressure Phase Equilibria and Modeling	MCC	M100C
Monday	3:15 PM	240	Solve this! Fundamental Approach to Problem Solving in Industrial Processes II (Invited Talks)*	MCC	101I

01J - Fluid Mechanics					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Sunday	3:30 PM	27	In Honor of Dennis Prieve's Retirement I (Invited Talks)*	MCC	101A
Monday	8:00 AM	81	Microfluidic and Nanoscale Flows: Separations & Particulates	Hilton	Conrad D
Monday	8:00 AM	92	Soft Matter Hydrodynamics	Hilton	Marquette I/II/III/ VIII/IX
Monday	12:30 PM	148	Hydrodynamics of Biological Systems	Hilton	Marquette I/II/III/ VIII/IX
Monday	12:30 PM	150	In Honor of Dennis Prieve's Retirement II (Invited Talks)*	MCC	M100B
Monday	12:30 PM	160	Microfluidic and Nanoscale Flows: Multiphase and Fields	Hilton	Conrad D
Monday	3:15 PM	234	Poster Session: Fluid Mechanics	Hilton	Marquette I/II/III/ VIII/IX

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01J - Fluid Mechanics (continued)					
Tuesday	8:00 AM	289	Hydrodynamics of Active Systems	Hilton	Conrad D
Tuesday	8:00 AM	296	Interfacial and Nonlinear Flows: Fluid Instabilities	Hilton	Marquette I/II/III/ VIII/IX
Tuesday	12:30 PM	369	Interfacial and Nonlinear Flows: Particle-Ladened Systems	Hilton	Marquette I/II/III/ VIII/IX
Tuesday	12:30 PM	380	Particulate and Multiphase Flows: Colloidal and Granular Systems	Hilton	Conrad D
Tuesday	3:15 PM	414	Colloidal Hydrodynamics: Structure and Microrheology	Hilton	Marquette I/II/III/ VIII/IX
Tuesday	3:15 PM	444	Particulate and Multiphase Flows: Dynamics of Emulsions, Bubbles, Droplets	Hilton	Conrad D
Wednesday	8:00 AM	468	Complex Fluids: Macromolecules	Hilton	Marquette I/II/III/ VIII/IX
Wednesday	8:00 AM	494	Multiphase Flow Characterization	Hilton	Conrad D
Wednesday	12:30 PM	535	Complex Fluids: Self & Directed Assembly	Hilton	Conrad D
Wednesday	12:30 PM	577	Turbulent and Reactive Flows	Hilton	Marquette I/II/III/ VIII/IX

02 - Separations Division					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Monday	8:00 AM	63	Division Plenary: Gerhold and Kunesh Awards on Separations (Invited Talks)	MCC	101F
Monday	12:30 PM	149	In Honor of Bill Koros I*	MCC	M100H
Monday	12:30 PM	152	In Honor of Stuart W. Churchill I (Invited Talks)*	MCC	101E
Monday	12:30 PM	159	Membrane Tutorial (Invited Talks)*	MCC	M100I
Monday	12:30 PM	173	Rapid Fire Session: TED-Sep Separations Division	MCC	M100G
Monday	12:30 PM	176	Solve this! Fundamental Approach to Problem Solving in Industrial Processes I (Invited Talks)*	MCC	101I
Monday	3:15 PM	227	In Honor of Bill Koros II*	MCC	M100H
Monday	3:15 PM	228	In Honor of Stuart W. Churchill II (Invited Talks)*	MCC	101E
Monday	3:15 PM	240	Solve this! Fundamental Approach to Problem Solving in Industrial Processes II (Invited Talks)*	MCC	101I
Tuesday	8:00 AM	292	In Honor of Bill Koros III*	MCC	M100H
Tuesday	12:30 PM	366	In Honor of Phil Wankat, the 2016 Recipient of the Warren K. Lewis Award (Invited Talks)*	MCC	205D
Tuesday	12:30 PM	387	Separation Process Improvements for Sustainability*	MCC	101C
Tuesday	3:15 PM	401	Poster Session: Separations Division	MCC	Exhibit Hall B
Wednesday	8:00 AM	462	Advances in Process Intensification: Enhanced Reactivity and Separations*	MCC	101E
Wednesday	3:15 PM	631	Survey Results and Best Practices: Laboratory Instruction (Invited Talks)*	MCC	205C

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02A - Distillation and Absorption					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Monday	12:30 PM	175	Refinery Distillation*	MCC	200A
Tuesday	8:00 AM	293	In Honor of Tony Cai of FRI	MCC	M100G
Tuesday	12:30 PM	329	Advances in Distillation Modelling	MCC	M100G
Wednesday	8:00 AM	474	Distillation Sequencing and Optimization	MCC	M100G
Wednesday	12:30 PM	520	Advances in Dividing Wall Towers	MCC	M100G
Wednesday	3:15 PM	605	HIDiC Applications and Reactive Distillation	MCC	M100G

02B - Crystallization and Evaporation					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Monday	12:30 PM	124	Area Plenary: Crystallization and Evaporation - Area 2B (Invited Talks)	MCC	M100J
Monday	3:15 PM	214	Continuous Crystallization Processes	MCC	M100J
Tuesday	8:00 AM	277	Crystallization Process Development*	MCC	102B
Tuesday	8:00 AM	310	Solid Form Selection: Cocrystals, Salts, Solvates, Polymorphs, and Beyond	MCC	M100J
Tuesday	12:30 PM	379	Particle Formation and Crystallization Processes from Liquids, Slurries, and Emulsions	MCC	M100J
Wednesday	8:00 AM	472	Crystallization of Pharmaceutical and Biological Molecules	MCC	M100J
Wednesday	12:30 PM	524	Amorphous and Crystalline Particle Engineering in Pharmaceuticals and Other Novel Materials	MCC	M100J
Wednesday	3:15 PM	612	Modeling and Control of Crystallization	MCC	M100J
Thursday	8:00 AM	683	Nucleation and Growth	MCC	M100J

02C - Extractions					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Wednesday	8:00 AM	479	Extractive Separations Fundamentals and Design	MCC	M100D
Wednesday	12:30 PM	540	Developments in Extractive Separations: Solvents	MCC	M100D
Wednesday	3:15 PM	597	Developments in Extractive Separations: Processes	MCC	M100D

02D - Membrane-Based Separations					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Monday	12:30 PM	149	In Honor of Bill Koros I	MCC	M100H
Monday	12:30 PM	158	Membranes for Bioseparations*	MCC	M100D
Monday	12:30 PM	159	Membrane Tutorial (Invited Talks)	MCC	M100I
Monday	3:15 PM	220	Fuel Cell Membranes	MCC	M100I
Monday	3:15 PM	227	In Honor of Bill Koros II	MCC	M100H
Monday	3:15 PM	235	Rapid Development and Implementation of Bioseparations*	MCC	M100D
Tuesday	8:00 AM	272	Charged Polymers for Membrane-Based Water and Energy Applications	MCC	M100I
Tuesday	8:00 AM	288	Highly Selective Separations with Membranes	MCC	M100D
Tuesday	8:00 AM	292	In Honor of Bill Koros III	MCC	M100H

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02D - Membrane-Based Separations (continued)					
Tuesday	12:30 PM	363	Industry Perspectives on Membrane Separations (Invited Talks)	MCC	M100H
Tuesday	12:30 PM	371	Membrane Modeling and Simulation	MCC	M100I
Tuesday	12:30 PM	387	Separation Process Improvements for Sustainability*	MCC	101C
Wednesday	8:00 AM	459	Advanced Inorganic Materials for Membrane Gas Separation - GS I	MCC	M100I
Wednesday	8:00 AM	514	Water Treatment, Desalination, and Reuse I	MCC	M100H
Wednesday	12:30 PM	562	Novel Polymeric Membranes - GS II	MCC	M100I
Wednesday	12:30 PM	580	Water Treatment, Desalination, and Reuse II	MCC	M100H
Wednesday	3:15 PM	608	Membrane Reactors	MCC	101D
Wednesday	3:15 PM	610	Mixed Matrix Membranes for Gas Separation - GS III	MCC	M100I
Wednesday	3:15 PM	635	Water Treatment, Desalination, and Reuse III	MCC	M100H
Thursday	8:00 AM	672	Membranes for CO_2 Separations - GS IV	MCC	M100I
Thursday	8:00 AM	691	Water Treatment, Desalination, and Reuse IV	MCC	M100H
Thursday	12:30 PM	694	Bioinspired Membranes and Membrane Processes	MCC	M100H
Thursday	12:30 PM	709	Diffusion in Polymers*	MCC	211D
Thursday	12:30 PM	722	Membrane Formation	MCC	M100I
Thursday	12:30 PM	728	Nanostructured and Self-Assembled Polymer Membranes	MCC	M100J
Thursday	3:15 PM	755	Membrane-Based Organic Solvent Separations	MCC	M100J
Thursday	3:15 PM	767	Surface Engineered and Responsive Membranes	MCC	M100H

02E - Adsorption and Ion Exchange					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Sunday	3:30 PM	25	Green Chemistry and Engineering*	MCC	101D
Monday	8:00 AM	84	Molecular Simulation of Surface, Interface and Confinement Effects - In Honor of Keith Gubbins' 80th Birthday I (Invited Talks)*	MCC	L100I
Monday	12:30 PM	122	Area Plenary: Adsorption and Ion Exchange I - In Honor of Douglas M. Ruthven (Invited Talks)	MCC	M100E
Monday	12:30 PM	147	Fundamental, Theory, and Model Development - In Honor of Keith Gubbins' 80th Birthday II (Invited Talks)*	MCC	L100H
Monday	3:15 PM	208	Area Plenary: Adsorption and Ion Exchange II	MCC	M100E
Tuesday	8:00 AM	253	Adsorbent Materials	MCC	M100E
Tuesday	8:00 AM	276	CO_2 Capture By Adsorption I: Process and Storage	MCC	M100F
Tuesday	12:30 PM	341	Chromatographic Separations and SMB	MCC	M100E
Tuesday	12:30 PM	345	CO_2 Capture By Adsorption II: Adsorbents	MCC	M100F
Tuesday	3:15 PM	397	Poster Session: Fundamentals and Applications of Adsorption and Ion Exchange	MCC	Exhibit Hall B
Wednesday	8:00 AM	458	Adsorption Applications for Sustainable Energy and Chemicals	MCC	M100F
Wednesday	12:30 PM	519	Adsorbent Materials for Sustainable Energy and Chemicals	MCC	M100F
Wednesday	12:30 PM	532	Characterization of Adsorbent Materials	MCC	M100E

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02E - Adsorption and Ion Exchange (continued)					
Wednesday	3:15 PM	614	Molecular Simulation of Adsorption I - In Honor of Keith Gubbins' 80th Birthday III (Invited Talks)	MCC	M100E
Wednesday	3:15 PM	628	PSA/TSA	MCC	M100F
Thursday	8:00 AM	660	Experimental Methods in Adsorption	MCC	M100D
Thursday	8:00 AM	682	Molecular Simulation of Adsorption II	MCC	M100E
Thursday	12:30 PM	710	Diffusion, Transport and Dynamics in Adsorption Systems	MCC	M100E
Thursday	3:15 PM	739	Adsorbent Materials: MOFs	MCC	M100I

02F - Fluid-Particle Separations					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Monday	3:15 PM	206	Advances in Fluid Particle Separations	MCC	M100G

02G - Fluid-Particle Separations					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Monday	12:30 PM	158	Membranes for Bioseparations	MCC	M100D
Monday	3:15 PM	235	Rapid Development and Implementation of Bioseparations	MCC	M100D
Thursday	8:00 AM	665	Innovations in Biopharmaceutical Discovery, Development, and Manufacturing*	MCC	204A/B

02H - Fluid-Particle Separations					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Tuesday	3:15 PM	399	Poster Session: General Topics on Separations	MCC	Exhibit Hall B

03 - Particle Technology Forum					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Sunday	3:30 PM	14	Amorphous Solid Dispersions for Drug Product*	MCC	205A/B
Monday	12:30 PM	152	In Honor of Stuart W. Churchill I (Invited Talks)*	MCC	101E
Monday	12:30 PM	176	Solve this! Fundamental Approach to Problem Solving in Industrial Processes I (Invited Talks)*	MCC	101I
Monday	3:15 PM	228	In Honor of Stuart W. Churchill II (Invited Talks)*	MCC	101E
Monday	3:15 PM	240	Solve this! Fundamental Approach to Problem Solving in Industrial Processes II (Invited Talks)*	MCC	101I
Tuesday	3:15 PM	400	Poster Session: Particle Technology Forum	MCC	Exhibit Hall B
Wednesday	3:15 PM	620	Particle Technology Awards Lectures	MCC	200H
Friday	8:00 AM	776	Particle Engineering As Applied to Pharmaceutical Formulations*	MCC	101D

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03A - Particle Production and Characterization

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	13	Agglomeration and Granulation Processes	MCC	200H
Monday	8:00 AM	60	Characterization of Engineered Particles and Nanostructured Particulate Systems	MCC	200H
Monday	12:30 PM	137	Control and Optimization of Particle and Solids Production	MCC	200H
Monday	3:15 PM	233	Population Balance Modeling for Particle Formation Processes: Nucleation, Aggregation, and Breakage Kernels	MCC	200H
Tuesday	8:00 AM	281	Dynamics and Modeling of Particles, Crystals and Agglomerate Formation	MCC	200H
Tuesday	12:30 PM	378	Particle Breakage and Comminution Processes	MCC	200H
Tuesday	12:30 PM	379	Particle Formation and Crystallization Processes from Liquids, Slurries, and Emulsions*	MCC	M100J
Tuesday	3:15 PM	443	Particle Engineering and Design for Product Value Enhancement	MCC	200H

03B -Fluidization and Fluid-Particle Systems

Day	Time	Session #	Session Title	Property	Room
Monday	8:00 AM	74	Fundamentals of Fluidization I	MCC	200I
Monday	12:30 PM	146	Fundamentals of Fluidization II	MCC	200I
Monday	3:15 PM	223	Fundamentals of Fluidization III: Experimental Findings	MCC	200I
Tuesday	8:00 AM	285	Fluid-Particle Flow and Reaction Systems I - In Honor of Professor L.S. Fan	MCC	200I
Tuesday	12:30 PM	356	Fluid-Particle Flow and Reaction Systems II - In Honor of Professor L.S. Fan	MCC	200I
Tuesday	3:15 PM	423	Fluidization and Fluid-Particle Systems for Energy and Environmental Applications I	MCC	200I
Wednesday	8:00 AM	480	Fluidization and Fluid-Particle Systems for Energy and Environmental Applications II	MCC	200I
Wednesday	12:30 PM	573	Special Session: Celebrating Prof. Mori's Career Long Accomplishments	MCC	200I
Thursday	8:00 AM	653	Circulating Fluidized Beds and Measurement Techniques in Fluid-Particle Systems	MCC	200I
Thursday	12:30 PM	716	Industrial Application of Computational and Numerical Approaches to Particle Flow I	MCC	200I
Thursday	3:15 PM	751	Industrial Application of Computational and Numerical Approaches to Particle Flow II	MCC	200I

03C -Solids Flow, Handling and Processing

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	21	Characterization and Measurement in Powder Processing	MCC	200I
Sunday	3:30 PM	43	Solids Handling and Processing in the Chemical Industry: What They Don't Teach You at School	MCC	200J
Monday	8:00 AM	65	Dynamics and Modeling of Particulate Systems I	MCC	200J
Monday	12:30 PM	139	Dynamics and Modeling of Particulate Systems II	MCC	200J

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03C -Solids Flow, Handling and Processing (continued)

Monday	3:15 PM	239	Solids Handling and Processing I	MCC	200J
Tuesday	8:00 AM	277	Crystallization Process Development*	MCC	102B
Tuesday	8:00 AM	311	Solids Handling and Processing II	MCC	200J
Wednesday	8:00 AM	486	Honoring the Lifelong Achievements of Dr. Jerry Johanson	MCC	200J
Thursday	8:00 AM	673	Mixing and Segregation of Particulate Systems I	MCC	200J
Thursday	12:30 PM	723	Mixing and Segregation of Particulate Systems II	MCC	200J

03D -Energetics

Day	Time	Session #	Session Title	Property	Room
Wednesday	12:30 PM	546	Energetic and Reactive Materials	MCC	200J
Wednesday	3:15 PM	632	Thermophysics and Reactions in Energetic Materials	MCC	200J

04 -Education

Day	Time	Session #	Session Title	Property	Room
Sunday	1:00 PM	7	Meet the Faculty Candidate Poster Session*	MCC	Exhibit Hall B
Sunday	3:30 PM	46	Workshop: Effective Teaching for New or Prospective Faculty	MCC	205C
Monday	12:30 PM	152	In Honor of Stuart W. Churchill I (Invited Talks)*	MCC	101E
Monday	12:30 PM	176	Solve this! Fundamental Approach to Problem Solving in Industrial Processes I (Invited Talks)*	MCC	101I
Monday	12:30 PM	181	Undergraduate Engineering Education of Ethics*	MCC	L100G
Monday	3:15 PM	228	In Honor of Stuart W. Churchill II (Invited Talks)*	MCC	101E
Monday	3:15 PM	240	Solve this! Fundamental Approach to Problem Solving in Industrial Processes II (Invited Talks)*	MCC	101I
Tuesday	12:30 PM	348	Digital Natives and Digital Tools: Teaching to Millennials with Technology	MCC	205C
Tuesday	12:30 PM	366	In Honor of Phil Wankat, the 2016 Recipient of the Warren K. Lewis Award (Invited Talks)	MCC	205D
Tuesday	12:30 PM	370	K-12 Outreach Activities and Other Broader Impacts	MCC	101I
Tuesday	3:15 PM	396	Poster Session: Chemical Engineering Education	MCC	Exhibit Hall B
Tuesday	3:15 PM	404	Broadening Participation in Chemical Engineering: Outreach Efforts that Work	MCC	101I
Wednesday	3:15 PM	636	Workshop: Best Practices in Advising and Mentoring Undergraduate and Graduate Students	MCC	205D

04A - Undergraduate Education

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	47	Workshop: Inexpensive Microcontrollers in Any ChE Course	MCC	205D
Monday	12:30 PM	145	Free Forum on Engineering Education: Junior and Senior Years I	MCC	205C
Monday	12:30 PM	154	Jumpstart Your Teaching!: Small Teaching Ideas for Course Improvement	MCC	205D
Monday	3:15 PM	213	ChE Potpourri: Beer and Thermodynamics	MCC	205D
Monday	3:15 PM	219	Free Forum on Engineering Education: Junior and Senior Years II	MCC	205C
Monday	3:15 PM	243	Use the FE Exam As an Assessment Tool?*	MCC	L100G

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04A - Undergraduate Education (continued)					
Tuesday	8:00 AM	309	Scholarship of Teaching and Learning and Assessment	MCC	205C
Tuesday	8:00 AM	312	Steal This Activity/Demonstration/Assignment	MCC	205D
Tuesday	11:00 AM	280	Diversity and Inclusion: Starting and Thriving in the Workplace (Invited Talks)	MCC	101G
Wednesday	12:30 PM	518	ABET Updates and Insights (Invited Talks)	MCC	205C
Wednesday	12:30 PM	552	Free Forum on Engineering Education: First Year and Sophomore Year	MCC	205D
Wednesday	3:15 PM	631	Survey Results and Best Practices: Laboratory Instruction (Invited Talks)	MCC	205C

04B - Graduate Education					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Wednesday	12:30 PM	563	NSF Workshop I: Highlights from CBET	MCC	101H
Wednesday	3:15 PM	619	NSF Workshop II: Proposal Writing and Discussions with Program Managers	MCC	101H

04A - Undergraduate Education					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Monday	8:00 AM	97	The Road Less Traveled: Professional Development for Teaching-Focused Faculty (Invited Talks)	MCC	205C

04I - Student Chapters Committee Liaison					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Sunday	12:30 PM	6	Chem-E-Car Competition	MCC	Exhibit Hall C
Monday	8:30 AM	101	Student Design Competition	MCC	103F
Monday	8:30 AM	102	Student Paper Competition	MCC	103E

04M - Young Faculty Forum					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Sunday	10:00 AM	5	Workshop: Career Planning for Prospective Faculty	MCC	101A
Wednesday	8:00 AM	515	Young Faculty Forum (Invited Talks)	MCC	205D

05 - Management Division					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Monday	12:30 PM	176	Solve this! Fundamental Approach to Problem Solving in Industrial Processes I (Invited Talks)*	MCC	101I
Monday	3:15 PM	240	Solve this! Fundamental Approach to Problem Solving in Industrial Processes II (Invited Talks)*	MCC	101I
Tuesday	12:30 PM	330	Applied Project Management Fundamentals: A Tutorial	MCC	L100G
Tuesday	12:30 PM	348	Digital Natives and Digital Tools: Teaching to Millennials with Technology*	MCC	205C
Tuesday	3:15 PM	432	Innovation from Beginning to End: Generating Ideas, Working with People, and Managing Projects	MCC	L100G

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06 - North American Mixing Forum					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Monday	8:00 AM	87	Novel Mixer and Mixed Reactor Design	MCC	102D
Monday	12:30 PM	152	In Honor of Stuart W. Churchill I (Invited Talks)*	MCC	101E
Monday	12:30 PM	161	Mixing in Multi-Phase Systems	MCC	102D
Monday	12:30 PM	176	Solve this! Fundamental Approach to Problem Solving in Industrial Processes I (Invited Talks)*	MCC	101I
Monday	3:15 PM	228	In Honor of Stuart W. Churchill II (Invited Talks)*	MCC	101E
Monday	3:15 PM	230	Mixing in Rheologically Complex Fluids	MCC	102D
Monday	3:15 PM	240	Solve this! Fundamental Approach to Problem Solving in Industrial Processes II (Invited Talks)*	MCC	101I
Tuesday	8:00 AM	298	Mixing in Single Phase Systems	MCC	102D
Tuesday	12:30 PM	393	The Use of CFD in Simulation of Mixing Processes	MCC	102D
Tuesday	3:15 PM	452	The Use of CFD in Simulation of Multiphase Mixing Processes	MCC	102D
Wednesday	8:00 AM	493	Mixing Scale-Up/Scale-Down Issues in Pharmaceutical and Biopharmaceuticals Processes	MCC	102D
Wednesday	3:15 PM	611	Mixing Award Session	MCC	102D

07 - Transport and Energy Processes					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Sunday	3:30 PM	40	Rechargeable / Secondary Battery Technologies for Energy Storage	MCC	200F
Monday	8:00 AM	48	Advanced Fuel Cell, Hydrogen Generation & Storage Technologies	MCC	200F
Monday	12:30 PM	152	In Honor of Stuart W. Churchill I (Invited Talks)	MCC	101E
Monday	12:30 PM	168	PEM (Polymer Electrolyte Membrane or Proton Exchange Membrane) Fuel Cells, DMFC (Direct Methanol Fuel Cells), and Alkaline Fuel Cells	MCC	200F
Monday	12:30 PM	176	Solve this! Fundamental Approach to Problem Solving in Industrial Processes I (Invited Talks)*	MCC	101I
Monday	3:15 PM	221	Fuel Cells, Electrolyzers, and Electrochemical Devices	MCC	200F
Monday	3:15 PM	228	In Honor of Stuart W. Churchill II (Invited Talks)	MCC	101E
Monday	3:15 PM	240	Solve this! Fundamental Approach to Problem Solving in Industrial Processes II (Invited Talks)*	MCC	101I
Tuesday	8:00 AM	257	Advances in Process Intensification: Enhanced Mass Transfer*	MCC	101E
Tuesday	8:00 AM	258	Alternative Fuels including Biofuels, Hydrogen, Renewable Hydrogen, and Syngas	MCC	200F
Tuesday	8:00 AM	315	Symposium on Solar Power and Chemical Systems in Honor of Prof. Edward A. Fletcher I*	MCC	201A/B
Tuesday	12:30 PM	346	CO_2 Capture, Utilization, and Disposal: Key to Clean Energy Production I	MCC	200F
Tuesday	12:30 PM	389	Symposium on Solar Power and Chemical Systems in Honor of Prof. Edward A. Fletcher II*	MCC	201A/B
Tuesday	3:15 PM	402	Poster Session: Transport and Energy Processes	MCC	Exhibit Hall B
Tuesday	3:15 PM	449	Symposium on Solar Power and Chemical Systems in Honor of Prof. Edward A. Fletcher III*	MCC	201A/B

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07 - Transport and Energy Processes (continued)					
Wednesday	8:00 AM	471	CO_2 Capture, Utilization, and Disposal: Key to Clean Energy Production II	MCC	200F
Wednesday	12:30 PM	550	Experimental, Theoretical, and Numerical Analysis of Transport Processes in Flow Reactors	MCC	200F
Wednesday	3:15 PM	602	Fate, Transport, and Remediation of Contaminants in the Environment	MCC	200F
Wednesday	3:15 PM	624	Process Intensification By Enhanced Heat and Mass Transfer*	MCC	101E

08 - Materials Engineering and Sciences Division					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Monday	8:00 AM	30	Materials Innovations Inspired By Acrivos Award Winner Chris Jones I	MCC	211A
Monday	12:30 PM	79	Materials Innovations Inspired By Acrivos Award Winner Chris Jones II	MCC	211A
Monday	12:30 PM	152	In Honor of Stuart W. Churchill I (Invited Talks)*	MCC	101E
Monday	12:30 PM	176	Solve this! Fundamental Approach to Problem Solving in Industrial Processes I (Invited Talks)*	MCC	101I
Monday	3:15 PM	222	Fuels from the Sun: Nanomaterials for Water Splitting, Artificial Photosynthesis, and Other Photocatalytic, and Photoelectrochemical Reactions*	MCC	200G
Monday	3:15 PM	228	In Honor of Stuart W. Churchill II (Invited Talks)*	MCC	101E
Monday	3:15 PM	240	Solve this! Fundamental Approach to Problem Solving in Industrial Processes II (Invited Talks)*	MCC	101I
Tuesday	3:15 PM	440	Nanomaterials for Light Harvesting and Novel Photophysical Phenomenon I*	MCC	200G
Wednesday	8:00 AM	475	Division Plenary: Materials Engineering & Sciences Division (Invited Talks)	MCC	211B

08A - Polymers					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Sunday	3:30 PM	36	Polymer Reaction Engineering	MCC	211B
Monday	8:00 AM	51	Area Plenary: Area 8A Emerging Areas in Polymer Science and Engineering I (Invited Talks)	MCC	211B
Monday	12:30 PM	123	Area Plenary: Area 8A Emerging Areas in Polymer Science and Engineering II (Invited Talks)	MCC	211B
Monday	3:15 PM	196	Poster Session: Materials Engineering & Sciences (08A - Polymers)*	MCC	Exhibit Hall B
Tuesday	8:00 AM	265	Biomacromolecular Gels	MCC	211B
Tuesday	8:00 AM	272	Charged Polymers for Membrane-Based Water and Energy Applications*	MCC	M100I
Tuesday	8:00 AM	303	Nanoscale Structure in Polymers	MCC	211C
Tuesday	8:00 AM	306	Polymer Processing and Rheology	MCC	211D
Tuesday	12:30 PM	354	Excellence in Graduate Polymer Research (Invited Talks)	MCC	211D
Tuesday	12:30 PM	364	Inhomogeneous Polymers	MCC	211B
Tuesday	12:30 PM	381	Polymer Networks and Gels	MCC	211C
Tuesday	3:15 PM	413	Charged and Ion-Containing Polymers	MCC	211B

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08A - Polymers (continued)					
Tuesday	3:15 PM	441	Nanoscale Phenomena in Macromolecular Systems	MCC	211C
Wednesday	12:30 PM	538	Conjugated Polymers	MCC	211C
Wednesday	12:30 PM	576	Thin Film Block Copolymer Self-Assembly and Morphology	MCC	211B
Wednesday	3:15 PM	621	Polymer Crystallization	MCC	211C
Wednesday	3:15 PM	622	Polymers for Energy Storage and Conversion	MCC	211D
Thursday	8:00 AM	680	Polymer Thin Films and Interfaces	MCC	211C
Thursday	8:00 AM	689	Thermodynamics of Polymers	MCC	211B
Thursday	12:30 PM	709	Diffusion in Polymers	MCC	211D
Thursday	12:30 PM	721	Mechanics and Structure in Polymers	MCC	211B
Thursday	12:30 PM	726	Multiscale and Coarse-Grained Modeling of Polymers	MCC	211C
Thursday	12:30 PM	728	Nanostructured and Self-Assembled Polymer Membranes*	MCC	M100J
Thursday	3:15 PM	740	Atomistic and Molecular Modeling and Simulation of Polymers	MCC	102A
Thursday	3:15 PM	758	Nanostructured Polymer Films	MCC	102D
Thursday	3:15 PM	766	Structure and Properties in Polymers	MCC	102E
Friday	8:00 AM	769	Bio-Based Polymers	MCC	102A
Friday	8:00 AM	777	Polymers in Additive Manufacturing	MCC	102D

08B - Biomaterials					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Sunday	3:30 PM	16	Biomaterials for Nucleic Acid Delivery	MCC	211C
Sunday	3:30 PM	17	Bionanotechnology for Gene and Drug Delivery I*	MCC	212A/B
Sunday	3:30 PM	31	Modeling of Biomaterials	MCC	211D
Monday	8:00 AM	55	Biomaterials: Faculty Candidates	MCC	211C
Monday	8:00 AM	85	Nanomaterials for Biological Applications I*	MCC	200G
Monday	8:00 AM	98	Topical Plenary: Advanced Biomaterials, Biofuels, and Biorefinery (Invited Talks)*	MCC	200E
Monday	12:30 PM	126	Area Plenary: Leaders in Biomaterials (Invited Talks)	MCC	211C
Monday	3:15 PM	197	Poster Session: Materials Engineering & Sciences (08B - Biomaterials)*	MCC	Exhibit Hall B
Tuesday	8:00 AM	267	Biomaterial Scaffolds for Tissue Engineering I: Anisotropic Materials	MCC	209A/B
Tuesday	12:30 PM	334	Biomaterial Scaffolds for Tissue Engineering II: Bioactive and Drug-Eluting Materials	MCC	209A/B
Tuesday	3:15 PM	411	Biomaterials: Graduate Student Award Session	MCC	211D
Tuesday	3:15 PM	426	Hydrogel Biomaterials	MCC	209A/B
Wednesday	8:00 AM	496	Nanotechnology for Biotechnology and Pharmaceuticals*	MCC	212A/B
Wednesday	12:30 PM	525	Biomaterials for Drug Delivery I: Particle Based Drug Delivery	MCC	209A/B
Wednesday	12:30 PM	526	Biomaterials for Immunological Applications I: Immune Activation and Vaccination	MCC	211A
Wednesday	12:30 PM	545	Emerging Applications of Cellulose Nanofibrils (CNFs) and Its Composites*	MCC	200B
Wednesday	3:15 PM	591	Biomaterials for Drug Delivery II: Micellar, Polymer and Protein Based Drug Carriers	MCC	211B

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08B - Biomaterials (continued)					
Wednesday	3:15 PM	592	Biomaterials for Immunological Applications II: Cancer Immunotherapy and Autoimmune Disease Treatments	MCC	211A
Wednesday	3:15 PM	593	Bioplastics, Biocomposites and Value-Added Uses of Biofuel Coproducts for Sustainable Manufacturing*	MCC	200B
Thursday	8:00 AM	647	Biomaterials for Drug Delivery III: Scaffolds Based Drug Delivery	MCC	210A/B
Thursday	8:00 AM	648	Biomaterials I: Instructive and Responsive Biomaterials	MCC	211A
Thursday	8:00 AM	686	Self-Assembled Biomaterials*	MCC	213A/B
Thursday	12:30 PM	696	Biomaterials II: Platforms for Cell Encapsulation, Isolation or Diagnostics	MCC	211A
Thursday	12:30 PM	729	Nanostructured Biomimetic and Biohybrid Materials and Devices*	MCC	213A/B
Thursday	3:15 PM	741	Biobased Materials: Design and Application*	MCC	103C
Thursday	3:15 PM	742	Biomimetic Materials I: Design and Synthesis	MCC	102F
Friday	8:00 AM	770	Biomaterials for in vitro Tissue Models and Improved Therapeutic Strategies	MCC	102E
Friday	8:00 AM	771	Biomimetic Materials II: Applications	MCC	102F

08D - Inorganic Materials					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Sunday	3:30 PM	9	Accelerated Discovery and Development of Inorganic Materials	MCC	209A/B
Monday	8:00 AM	96	Synthesis and Application of Porous Materials I: Synthesis and Characterization	MCC	209A/B
Monday	12:30 PM	177	Synthesis and Application of Porous Materials II: Application	MCC	209A/B
Monday	3:15 PM	198	Poster Session: Materials Engineering & Sciences (08D - Inorganic Materials)*	MCC	Exhibit Hall B
Wednesday	3:15 PM	617	Nanostructured Thin Films	MCC	209A/B
Thursday	8:00 AM	687	Templated Assembly of Inorganic Nanomaterials	MCC	209A/B
Thursday	12:30 PM	725	MOFs, COFs, and Porous Polymer Materials I: Synthesis	MCC	209A/B
Thursday	12:30 PM	735	Semiconducting Quantum Dots I: Surface Chemistry and Assemblies*	MCC	210A/B
Thursday	3:15 PM	757	MOFs, COFs, and Porous Polymer Materials II: Application	MCC	102C
Thursday	3:15 PM	765	Semiconducting Quantum Dots II: Novel Syntheses and Devices*	MCC	102B

08E - Electronics and Photonics					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Sunday	3:30 PM	34	Organic, Polymeric, and Hybrid Semiconductors	MCC	210A/B
Sunday	3:30 PM	167	Nanomaterials Synthesis and Self-Assembly Strategies	MCC	211A
Monday	8:00 AM	78	Materials for Electrochemical Energy I	MCC	210A/B
Monday	12:30 PM	157	Materials for Electrochemical Energy II	MCC	210A/B
Monday	3:15 PM	199	Poster Session: Materials Engineering & Sciences (08E - Electronic and Photonic Materials)*	MCC	Exhibit Hall B
Monday	3:15 PM	222	Fuels from the Sun: Nanomaterials for Water Splitting, Artificial Photosynthesis, and Other Photocatalytic, and Photoelectrochemical Reactions*	MCC	200G

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08E - Electronics and Photonics (continued)					
Tuesday	8:00 AM	262	Area 8E Graduate Student Award Finalists	MCC	211A
Tuesday	8:00 AM	301	Nanomaterials for Energy Storage*	MCC	200G
Tuesday	12:30 PM	375	Nanoelectronic and Photonic Materials I: Nanoscale Applications	MCC	211A
Tuesday	12:30 PM	376	Nanomaterials for Hydrogen Production and Fuel Cells*	MCC	200G
Tuesday	3:15 PM	439	Nanoelectronic and Photonic Materials II: 2D Materials	MCC	211A
Tuesday	3:15 PM	440	Nanomaterials for Light Harvesting and Novel Photophysical Phenomenon I*	MCC	200G
Wednesday	3:15 PM	604	Halide Perovskite Synthesis and Applications	MCC	210A/B
Wednesday	3:15 PM	617	Nanostructured Thin Films*	MCC	209A/B
Thursday	12:30 PM	735	Semiconducting Quantum Dots I: Surface Chemistry and Assemblies	MCC	210A/B
Thursday	3:15 PM	765	Semiconducting Quantum Dots II: Novel Syntheses and Devices	MCC	102B
Friday	8:00 AM	775	Nanostructured/Thin Film Photovoltaics	MCC	102B

08F - Composites					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Monday	8:00 AM	59	Characterization of Composites	MCC	211D
Monday	12:30 PM	774	Multifunctional Composites	MCC	211D
Monday	3:15 PM	200	Poster Session: Materials Engineering & Sciences (08F - Composite Materials)*	MCC	Exhibit Hall B
Wednesday	12:30 PM	536	Composites for Environmental Applications	MCC	211D
Thursday	8:00 AM	640	2D Nanocomposites: New Composites with 2-Dimensional Nanomaterials	MCC	211D
Friday	8:00 AM	118	Advanced Structural Composites	MCC	102C

09 - Environmental Division					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Monday	12:30 PM	121	Applied Environmental Catalysis I*	MCC	L100B
Monday	12:30 PM	144	Environmental Division Awards and Honors (Invited Talks)	MCC	102E
Monday	12:30 PM	152	In Honor of Stuart W. Churchill I (Invited Talks)*	MCC	101E
Monday	12:30 PM	176	Solve this! Fundamental Approach to Problem Solving in Industrial Processes I (Invited Talks)*	MCC	101I
Monday	12:30 PM	178	The Food-Energy-Water Nexus*	MCC	102A
Monday	3:15 PM	207	Applied Environmental Catalysis II*	MCC	L100B
Monday	3:15 PM	228	In Honor of Stuart W. Churchill II (Invited Talks)*	MCC	101E
Monday	3:15 PM	240	Solve this! Fundamental Approach to Problem Solving in Industrial Processes II (Invited Talks)*	MCC	101I
Tuesday	8:00 AM	273	Combustion Kinetics and Emissions I*	MCC	L100F
Tuesday	8:00 AM	302	Nanoparticles and Health*	MCC	210A/B
Tuesday	8:00 AM	314	Sustainable Management of Post Consumption/Use Biomaterials*	MCC	101C
Tuesday	12:30 PM	342	Combustion Kinetics and Emissions II*	MCC	L100F
Tuesday	12:30 PM	353	Environmental Implications of Nanomaterials: Biological Interactions*	MCC	210A/B
Tuesday	12:30 PM	368	Integrated Process Engineering and Economics Analysis*	MCC	103B

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09 - Environmental Division (continued)					
Tuesday	12:30 PM	388	Structure in the Design of Sustainable Processes and Supply Chains*	MCC	102A
Wednesday	8:00 AM	478	Environmental Applications of Nanotechnology and Nanomaterials I*	MCC	210A/B
Wednesday	8:00 AM	487	Important Issues in Professional Development Including the Management Division's Award Recipient Presentation (Invited Talks)*	MCC	L100G
Wednesday	12:30 PM	536	Composites for Environmental Applications*	MCC	211D
Wednesday	3:15 PM	583	Poster Session: Environmental Division	MCC	Exhibit Hall B
Wednesday	4:45 PM	637	Rapid Fire Session: Environmental Division	MCC	102E

09A - Air					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Sunday	3:30 PM	33	Novel Materials for Environmental Applications	MCC	102C
Tuesday	8:00 AM	263	Atmospheric Chemistry and Physics I	MCC	102F
Tuesday	8:00 AM	302	Nanoparticles and Health*	MCC	210A/B
Tuesday	12:30 PM	333	Atmospheric Chemistry and Physics II	MCC	102F

09B - Water					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Monday	8:00 AM	49	Advanced Oxidation Processes I	MCC	102F
Monday	3:15 PM	205	Advanced Oxidation Processes II	MCC	102F
Wednesday	8:00 AM	460	Advanced Treatment for Water Reuse and Recycling	MCC	102F
Wednesday	8:00 AM	514	Water Treatment, Desalination, and Reuse I*	MCC	M100H
Wednesday	12:30 PM	580	Water Treatment, Desalination, and Reuse II*	MCC	M100H
Wednesday	3:15 PM	635	Water Treatment, Desalination, and Reuse III*	MCC	M100H
Thursday	8:00 AM	655	Community-Based Water Treatment Innovations	MCC	102F
Thursday	8:00 AM	691	Water Treatment, Desalination, and Reuse IV*	MCC	M100H

09B - Solid and Hazardous Waste					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Tuesday	12:30 PM	359	Fundamentals and Applications for Hazardous Waste Treatment	MCC	102E
Tuesday	3:15 PM	424	Fundamentals and Applications for Municipal Solid Waste Treatment and Valorization	MCC	102E
Wednesday	8:00 AM	477	Environmental Advances in Nuclear and Hazardous Waste Treatment I	MCC	102E
Wednesday	12:30 PM	548	Environmental Advances in Nuclear and Hazardous Waste Treatment II	MCC	102E

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09D - Process Development					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Wednesday	12:30 PM	521	Advances in Life Cycle Optimization for Process Development	MCC	102F

09F - Fundamentals					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Monday	8:00 AM	73	Fundamentals of Environmental Kinetics and Reaction Engineering	MCC	102E
Monday	3:15 PM	224	Fundamentals of Food, Energy, and Water Systems	MCC	102A
Tuesday	12:30 PM	388	Structure in the Design of Sustainable Processes and Supply Chains	MCC	102A

09G - Sustainability					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Tuesday	8:00 AM	313	Sustainable Fuel from Renewable Resources	MCC	102E
Tuesday	3:15 PM	427	CO_2 Industrial, Engineering and R&D Approaches	MCC	102C
Thursday	8:00 AM	662	Going to a Decision Point in Sustainability Analysis	MCC	102E
Thursday	12:30 PM	737	Sustainability Metrics at the Process and Product Level	MCC	102E

09H - Climate Change					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Tuesday	3:15 PM	412	Carbon Dioxide Capture Technologies and Their Use	MCC	102F

10 - Computing Systems and Technology Division					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Sunday	3:30 PM	19	CAST Director's Student Presentation Award Finalists	MCC	103D
Monday	8:00 AM	61	Division Plenary: CAST (Invited Talks)	MCC	103C
Monday	12:30 PM	152	In Honor of Stuart W. Churchill I (Invited Talks)*	MCC	101E
Monday	12:30 PM	176	Solve this! Fundamental Approach to Problem Solving in Industrial Processes I (Invited Talks)*	MCC	101I
Monday	12:30 PM	180	Tools for Product Design*	MCC	102B
Monday	3:15 PM	228	In Honor of Stuart W. Churchill II (Invited Talks)*	MCC	101E
Monday	3:15 PM	240	Solve this! Fundamental Approach to Problem Solving in Industrial Processes II (Invited Talks)*	MCC	101I
Monday	4:45 PM	246	CAST Rapid Fire Session I	MCC	103C
Monday	4:45 PM	247	CAST Rapid Fire Session II	MCC	103D
Monday	4:45 PM	248	CAST Rapid Fire Session III	MCC	103E
Monday	4:45 PM	249	CAST Rapid Fire Session IV	MCC	103F
Tuesday	8:00 AM	300	Multiscale Systems Engineering I - In Honor of Professor Christodoulos A. Floudas (Invited Talks)	MCC	103C
Tuesday	12:30 PM	368	Integrated Process Engineering and Economics Analysis*	MCC	103B
Tuesday	12:30 PM	374	Multiscale Systems Engineering II - In Honor of Professor Christodoulos A. Floudas (Invited Talks)	MCC	103C

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10 - Computing Systems and Technology Division (continued)					
Tuesday	3:15 PM	437	Modeling & Simulation of Complex Systems*	MCC	103A
Tuesday	3:15 PM	448	Software Tools and Implementations for Process Systems Engineering	MCC	103E

10A - Systems and Process Design

Day	Time	Session #	Session Title	Property	Room
Monday	12:30 PM	171	Process Design	MCC	103C
Monday	3:15 PM	189	Interactive Session: Systems and Process Design	MCC	Exhibit Hall B
Tuesday	8:00 AM	317	The Energy-Water Nexus*	MCC	102A
Tuesday	12:30 PM	384	Process Research & Innovation for Improved Process Efficiency*	MCC	102B
Tuesday	3:15 PM	419	Design Under Uncertainty	MCC	103C
Tuesday	3:15 PM	429	Industrial Innovations through Modeling and Optimization*	MCC	102B
Wednesday	8:00 AM	503	Process Intensification through Process Systems Engineering	MCC	101D
Wednesday	12:30 PM	547	Energy System Design I	MCC	103C
Wednesday	3:15 PM	601	Energy System Design II	MCC	103C
Thursday	8:00 AM	658	Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains I*	MCC	101E
Thursday	8:00 AM	666	Integrated Product and Process Design	MCC	103C
Thursday	8:00 AM	681	Process Design: Innovation for Sustainability*	MCC	101C
Thursday	12:30 PM	707	Design and Optimization of Environmentally Sustainable Advanced Fossil Energy Systems*	MCC	200C

10B - Systems and Process Control

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	12	Advances in Process Control	MCC	103E
Monday	12:30 PM	170	Process Control Applications	MCC	103D
Monday	3:15 PM	188	Interactive Session: Systems and Process Control	MCC	Exhibit Hall B
Tuesday	8:00 AM	284	Estimation and Control of Uncertain Systems	MCC	103D
Tuesday	12:30 PM	383	Process Modeling and Identification	MCC	103D
Tuesday	3:15 PM	416	Computational Methods in Biological and Biomedical Systems I*	MCC	103F
Tuesday	3:15 PM	430	In Honor of Christos Georgakis' 70th Birthday	MCC	103D
Wednesday	8:00 AM	497	Networked, Decentralized, and Distributed Control	MCC	103D
Wednesday	12:30 PM	564	Optimization and Predictive Control	MCC	103D
Wednesday	3:15 PM	599	Dynamic Simulation and Optimization*	MCC	103E
Wednesday	3:15 PM	606	In Honor of Jim Rawlings' 60th Birthday	MCC	103D
Wednesday	3:15 PM	612	Modeling and Control of Crystallization*	MCC	M100J
Wednesday	3:15 PM	625	Process Monitoring & Fault Detection*	MCC	103F
Thursday	8:00 AM	667	Integrated Production Scheduling and Control	MCC	103D
Thursday	12:30 PM	711	Dynamics, Reduction, and Control of Distributed Parameter Systems*	MCC	103F
Thursday	12:30 PM	712	Economics and Process Control	MCC	103C
Thursday	12:30 PM	724	Modeling, Control, and Optimization of Energy Systems I	MCC	103D
Thursday	3:15 PM	756	Modeling, Control and Optimization of Energy Systems II	MCC	103D

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10C - Computers in Operations and Information Processing

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	44	Supply Chain Logistics and Optimization	MCC	103F
Monday	12:30 PM	120	Advances in Optimization I	MCC	103E
Monday	3:15 PM	190	Interactive Session: Systems and Process Operations	MCC	Exhibit Hall B
Tuesday	3:15 PM	419	Design Under Uncertainty*	MCC	103C
Wednesday	8:00 AM	461	Advances in Optimization II	MCC	103E
Wednesday	12:30 PM	522	Advances in MINLP and Global Optimization	MCC	103E
Wednesday	12:30 PM	547	Energy System Design I*	MCC	103C
Wednesday	12:30 PM	564	Optimization and Predictive Control*	MCC	103D
Wednesday	3:15 PM	599	Dynamic Simulation and Optimization	MCC	103E
Thursday	8:00 AM	664	Industrial Applications in Design and Operations	MCC	103E
Thursday	8:00 AM	667	Integrated Production Scheduling and Control*	MCC	103D
Thursday	12:30 PM	733	Planning and Scheduling I	MCC	103E
Thursday	3:15 PM	761	Planning and Scheduling II	MCC	103E

10D - Applied Mathematics and Numerical Analysis

Day	Time	Session #	Session Title	Property	Room
Monday	12:30 PM	125	Area Plenary: Future Directions in Applied Mathematics and Numerical Analysis (Invited Talks)	MCC	103F
Monday	3:15 PM	186	Interactive Session: Applied Mathematics and Numerical Analysis	MCC	Exhibit Hall B
Tuesday	8:00 AM	254	Advances in Computational Methods and Numerical Analysis	MCC	103F
Tuesday	12:30 PM	343	Complex and Networked Chemical and Biochemical Systems	MCC	103F
Tuesday	3:15 PM	416	Computational Methods in Biological and Biomedical Systems I	MCC	103F
Wednesday	8:00 AM	470	Computational Methods in Biological and Biomedical Systems II	MCC	103F
Wednesday	8:00 AM	497	Networked, Decentralized, and Distributed Control*	MCC	103D
Wednesday	12:30 PM	558	Modeling and Computation in Energy and Environment	MCC	103F
Thursday	12:30 PM	711	Dynamics, Reduction, and Control of Distributed Parameter Systems	MCC	103F

10E - Data and Information Systems

Day	Time	Session #	Session Title	Property	Room
Monday	3:15 PM	187	Interactive Session: Data and Information Systems	MCC	Exhibit Hall B
Tuesday	8:00 AM	255	Advances in Data Analysis, Information Management, and Intelligent Systems I	MCC	103E
Tuesday	12:30 PM	328	Advances in Data Analysis, Information Management, and Intelligent Systems II	MCC	103E
Tuesday	3:15 PM	438	Multivariate Modeling and Quality-by-Control Approaches for Pharmaceutical Processes*	MCC	205A/B
Wednesday	12:30 PM	558	Modeling and Computation in Energy and Environment*	MCC	103F
Wednesday	3:15 PM	595	Data Mining and Machine Learning in Molecular Sciences I*	MCC	L100H
Wednesday	3:15 PM	625	Process Monitoring & Fault Detection	MCC	103F

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10E - Data and Information Systems (continued)					
Thursday	8:00 AM	646	Big Data in Process Modeling, Estimation and Control	MCC	103F
Thursday	3:15 PM	747	Data Mining and Machine Learning in Molecular Sciences II*	MCC	103A

12 - Process Development Division					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Sunday	3:30 PM	35	Panel Speakers Forum: Chemical Process and Product Careers in Academia Vs. Industry	MCC	102B
Monday	8:00 AM	88	Physical Properties for Chemical Process and Product Design*	MCC	102B
Monday	12:30 PM	152	In Honor of Stuart W. Churchill I (Invited Talks)*	MCC	101E
Monday	12:30 PM	176	Solve this! Fundamental Approach to Problem Solving in Industrial Processes I (Invited Talks)*	MCC	101I
Monday	12:30 PM	180	Tools for Product Design*	MCC	102B
Monday	3:15 PM	210	Best Practices in Pilot Plants*	MCC	102C
Monday	3:15 PM	228	In Honor of Stuart W. Churchill II (Invited Talks)*	MCC	101E
Monday	3:15 PM	240	Solve this! Fundamental Approach to Problem Solving in Industrial Processes II (Invited Talks)*	MCC	101I
Tuesday	8:00 AM	277	Crystallization Process Development*	MCC	102B
Tuesday	8:00 AM	278	Design, Construction and Operation of Unit Operations Labs and Pilot Plants*	MCC	102C
Tuesday	8:00 AM	312	Steal This Activity/Demonstration/Assignment*	MCC	205D
Tuesday	12:30 PM	368	Integrated Process Engineering and Economics Analysis*	MCC	103B
Tuesday	12:30 PM	382	Process Intensification By Process Integration*	MCC	101E
Tuesday	12:30 PM	384	Process Research & Innovation for Improved Process Efficiency*	MCC	102B
Tuesday	3:15 PM	408	Advances in Process Intensification*	MCC	101E
Tuesday	3:15 PM	429	Industrial Innovations through Modeling and Optimization*	MCC	102B
Wednesday	8:00 AM	502	Pharmaceutical Process Development and Pilot Plants*	MCC	102C
Wednesday	12:30 PM	567	Process Intensification through the Application of Microreactors and Membrane Reactors*	MCC	101E
Wednesday	12:30 PM	568	Process Scale-up Techniques*	MCC	102C
Wednesday	3:15 PM	586	Poster Session: Process Development	MCC	Exhibit Hall B
Wednesday	3:15 PM	624	Process Intensification By Enhanced Heat and Mass Transfer*	MCC	101E

12A - Process Research and Innovation					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Sunday	3:30 PM	18	Bioseparations and Downstream Processing*	MCC	206A/B
Sunday	3:30 PM	22	Cutting Edge and Innovative Corporate & Industrial Research Projects (Invited Talks)*	MCC	101H
Sunday	3:30 PM	35	Panel Speakers Forum: Chemical Process and Product Careers in Academia Vs. Industry*	MCC	102B
Monday	3:15 PM	215	Development of Sustainable New Materials and Intermediates	MCC	102B
Tuesday	8:00 AM	277	Crystallization Process Development	MCC	102B
Tuesday	12:30 PM	384	Process Research & Innovation for Improved Process Efficiency	MCC	102B

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12A - Process Research and Innovation (continued)					
Tuesday	3:15 PM	417	Conceptual Process Design in Refining, Petrochemicals and Gas Processing*	MCC	200A
Tuesday	3:15 PM	429	Industrial Innovations through Modeling and Optimization	MCC	102B

12B - Pilot Plants					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Sunday	3:30 PM	35	Panel Speakers Forum: Chemical Process and Product Careers in Academia Vs. Industry*	MCC	102B
Monday	3:15 PM	210	Best Practices in Pilot Plants	MCC	102C
Tuesday	8:00 AM	278	Design, Construction and Operation of Unit Operations Labs and Pilot Plants	MCC	102C
Tuesday	12:30 PM	368	Integrated Process Engineering and Economics Analysis*	MCC	103B
Wednesday	8:00 AM	502	Pharmaceutical Process Development and Pilot Plants	MCC	102C
Wednesday	12:30 PM	568	Process Scale-up Techniques	MCC	102C

12C - Technology Transfer and Manufacturing					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Sunday	3:30 PM	22	Cutting Edge and Innovative Corporate & Industrial Research Projects (Invited Talks)*	MCC	101H
Sunday	3:30 PM	35	Panel Speakers Forum: Chemical Process and Product Careers in Academia Vs. Industry*	MCC	102B
Monday	8:00 AM	91	Risk Reduction in- and Implementation of- Process & Technology Development	MCC	102C
Tuesday	12:30 PM	368	Integrated Process Engineering and Economics Analysis*	MCC	103B

12E - Process Intensification & Microprocess Engineering					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Sunday	3:30 PM	35	Panel Speakers Forum: Chemical Process and Product Careers in Academia Vs. Industry*	MCC	102B
Tuesday	12:30 PM	382	Process Intensification By Process Integration	MCC	101E
Tuesday	3:15 PM	408	Advances in Process Intensification	MCC	101E
Wednesday	8:00 AM	503	Process Intensification through Process Systems Engineering*	MCC	101D
Wednesday	12:30 PM	567	Process Intensification through the Application of Microreactors and Membrane Reactors	MCC	101E
Wednesday	3:15 PM	624	Process Intensification By Enhanced Heat and Mass Transfer	MCC	101E

12G - Product Design					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Sunday	3:30 PM	35	Panel Speakers Forum: Chemical Process and Product Careers in Academia Vs. Industry*	MCC	102B
Monday	8:00 AM	88	Physical Properties for Chemical Process and Product Design	MCC	102B
Monday	8:30 AM	101	Student Design Competition*	MCC	103F

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12G - Product Design (continued)					
Monday	12:30 PM	180	Tools for Product Design	MCC	102B
Monday	3:15 PM	215	Development of Sustainable New Materials and Intermediates*	MCC	102B
Thursday	8:00 AM	657	Critical Quality Attribute Monitoring and Control in Pharmaceutical Manufacturing I*	MCC	205C
Thursday	8:00 AM	666	Integrated Product and Process Design*	MCC	103C
Thursday	12:30 PM	705	Critical Quality Attribute Monitoring and Control in Pharmaceutical Manufacturing II*	MCC	205C
Thursday	3:15 PM	746	Critical Quality Attribute Monitoring and Control in Pharmaceutical Manufacturing III*	MCC	101D

14 - Nuclear Engineering Division					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Monday	12:30 PM	152	In Honor of Stuart W. Churchill I (Invited Talks)*	MCC	101E
Monday	12:30 PM	176	Solve this! Fundamental Approach to Problem Solving in Industrial Processes I (Invited Talks)*	MCC	101I
Monday	3:15 PM	185	Wilson Award Winner	MCC	200D
Monday	3:15 PM	228	In Honor of Stuart W. Churchill II (Invited Talks)*	MCC	101E
Monday	3:15 PM	240	Solve this! Fundamental Approach to Problem Solving in Industrial Processes II (Invited Talks)*	MCC	101I
Monday	4:00 PM	245	Solvent Extraction and Adsorption in Spent Fuel Reprocessing and Radioactive Waste Management	MCC	200D
Tuesday	8:00 AM	259	Applications of Chemical Engineering to Nuclear Materials	MCC	200D
Tuesday	12:30 PM	327	Advances in Chemical Separation Technologies in Nuclear Processes	MCC	200D
Tuesday	3:15 PM	407	Advances in Chemical and Nuclear Process Safety	MCC	200D
Wednesday	8:00 AM	477	Environmental Advances in Nuclear and Hazardous Waste Treatment I*	MCC	102E
Wednesday	8:00 AM	510	Theory, Modeling and Simulation of Nuclear Chemical Processes	MCC	200D
Wednesday	12:30 PM	548	Environmental Advances in Nuclear and Hazardous Waste Treatment II*	MCC	102E

15 - Food, Pharmaceutical & Bioengineering Division					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Monday	8:00 AM	76	In Honor of Martin Yarmush I (Invited Talks)	MCC	208C/D
Monday	8:00 AM	95	Sustainable Microbial Process for Food, Feeds, Energy, and Environment*	MCC	103B
Monday	12:30 PM	151	In Honor of Martin Yarmush II (Invited Talks)	MCC	208C/D
Monday	12:30 PM	152	In Honor of Stuart W. Churchill I (Invited Talks)*	MCC	101E
Monday	12:30 PM	176	Solve this! Fundamental Approach to Problem Solving in Industrial Processes I (Invited Talks)*	MCC	101I
Monday	3:15 PM	228	In Honor of Stuart W. Churchill II (Invited Talks)*	MCC	101E
Monday	3:15 PM	240	Solve this! Fundamental Approach to Problem Solving in Industrial Processes II (Invited Talks)*	MCC	101I
Tuesday	8:00 AM	294	In Honor of Wei-Shou Hu I - 30 Years of Mammalian Cell Culture Engineering for Biologics Manufacturing (Invited Talks)	MCC	208C/D

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15 - Food, Pharmaceutical & Bioengineering Division (continued)					
Tuesday	12:30 PM	367	In Honor of Wei-Shou Hu II - 30 Years of Mammalian Cell Culture Engineering for Biologics Manufacturing (Invited Talks)	MCC	208C/D
Tuesday	3:15 PM	421	Division Plenary: Food, Pharmaceutical, and Bioengineering Division (Invited Talks)	MCC	208C/D

15A - Food					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Monday	8:00 AM	50	Advances in Membrane Technologies for Food and Bioprocessing	MCC	206A/B
Monday	3:15 PM	194	Poster Session: Food and Bioprocess Engineering	MCC	Exhibit Hall B
Monday	3:15 PM	224	Fundamentals of Food, Energy, and Water Systems*	MCC	102A
Tuesday	8:00 AM	256	Advances in Functional Foods Production	MCC	206A/B
Wednesday	8:00 AM	491	Metabolic and Process Engineering for Value-Added Products from Food Processing	MCC	206A/B
Thursday	8:00 AM	642	Advances in Food and Bioprocess Engineering	MCC	206A/B

15B - Pharmaceuticals					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Sunday	3:30 PM	14	Amorphous Solid Dispersions for Drug Product*	MCC	205A/B
Sunday	3:30 PM	24	Green Chemical Reaction Engineering for Sustainability*	MCC	103A
Sunday	3:30 PM	26	Green Pharmaceutical Process Development and Biocatalysis*	MCC	204A/B
Monday	8:00 AM	71	Forum Plenary: Pharmaceutical Discovery, Development, and Manufacturing Forum (Invited Talks)*	MCC	205A/B
Monday	12:30 PM	162	Model Based Integrated Design of Pharmaceutical Drug Product Processes*	MCC	205A/B
Monday	3:15 PM	203	Poster Session: Pharmaceutical*	MCC	Exhibit Hall B
Monday	6:30 PM	251	Pharmaceutical Discovery, Development, and Manufacturing Forum Awards Ceremony*	MCC	205A/B
Tuesday	8:00 AM	274	Continuous Processing Technologies Applied in Drug Product Development*	MCC	204A/B
Tuesday	8:00 AM	299	Model Based Integrated Design of Pharmaceutical Drug Substance Processes I*	MCC	205A/B
Tuesday	8:00 AM	310	Solid Form Selection: Cocrystals, Salts, Solvates, Polymorphs, and Beyond*	MCC	M100J
Tuesday	12:30 PM	344	Continuous Processing Technologies Applied in Drug Product Manufacturing*	MCC	204A/B
Tuesday	12:30 PM	373	Model Based Integrated Design of Pharmaceutical Drug Substance Processes II*	MCC	205A/B
Tuesday	3:15 PM	418	Continuous Processing Technologies Applied in Drug Substance Development Chemistry*	MCC	204A/B
Tuesday	3:15 PM	438	Multivariate Modeling and Quality-by-Control Approaches for Pharmaceutical Processes*	MCC	205A/B
Wednesday	8:00 AM	472	Crystallization of Pharmaceutical and Biological Molecules*	MCC	M100J
Wednesday	8:00 AM	500	Panel: Precompetitive Collaboration*	MCC	204A/B
Wednesday	8:00 AM	507	Reaction Engineering in Pharmaceuticals and Fine Chemicals*	MCC	L100B

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15B - Pharmaceuticals (continued)					
Wednesday	12:30 PM	529	Catalysis for Pharmaceuticals and Fine Chemicals*	MCC	L100B
Wednesday	12:30 PM	539	Continuous Processing Technologies Applied in Drug Substance Development Crystallization and Drying*	MCC	204A/B
Wednesday	12:30 PM	565	PAT for Process Understanding, Reduced Testing, and Elucidation of Fundamental Phenomena in Drug Product/Substance Development*	MCC	201A/B
Wednesday	3:15 PM	594	Continuous Processing Technologies Applied in Drug Substance Manufacturing*	MCC	204A/B
Wednesday	3:15 PM	596	Development of Processes and Products for Pharmaceuticals and Hybrid Therapeutics*	MCC	201A/B
Wednesday	3:15 PM	623	Process Intensification and Advanced Control of Pharmaceutical Processes*	MCC	101C
Thursday	8:00 AM	657	Critical Quality Attribute Monitoring and Control in Pharmaceutical Manufacturing I*	MCC	205C
Thursday	8:00 AM	665	Innovations in Biopharmaceutical Discovery, Development, and Manufacturing*	MCC	204A/B
Thursday	8:00 AM	671	Materials Science in Pharmaceutical Process Development I*	MCC	205D
Thursday	12:30 PM	705	Critical Quality Attribute Monitoring and Control in Pharmaceutical Manufacturing II*	MCC	205C
Thursday	12:30 PM	717	Innovative Technologies in Pharmaceutical Discovery, Manufacturing and Delivery*	MCC	204A/B
Thursday	12:30 PM	720	Materials Science in Pharmaceutical Process Development II*	MCC	205D
Thursday	3:15 PM	746	Critical Quality Attribute Monitoring and Control in Pharmaceutical Manufacturing III*	MCC	101D
Thursday	3:15 PM	762	Quality by Design in Drug Substance Process Development*	MCC	101E
Friday	8:00 AM	776	Particle Engineering As Applied to Pharmaceutical Formulations*	MCC	101D
Friday	8:00 AM	778	Quality by Design in Drug Product Formulation, Design, and Process Development*	MCC	101E

15C - Bioengineering					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Sunday	3:30 PM	15	Biobased Fuels and Chemicals: Biosynthetic Pathway Engineering & Enzymatic Conversion	MCC	208C/D
Sunday	3:30 PM	18	Bioseparations and Downstream Processing	MCC	206A/B
Monday	8:00 AM	67	Emerging Tools and Enabling Technologies in Synthetic Biology and Metabolic Engineering	MCC	207A/B
Monday	8:00 AM	75	Gene Regulation Engineering	MCC	208A
Monday	12:30 PM	119	Advances in Metabolic Engineering of Photosynthetic/Non-Model Organisms	MCC	206A/B
Monday	12:30 PM	142	Emerging Tools and Enabling Technologies in Synthetic Biology	MCC	207A/B
Monday	3:15 PM	191	Poster Session: Bioengineering	MCC	Exhibit Hall B
Tuesday	8:00 AM	291	In silico Systems Biology I: Biotechnology Applications	MCC	207A/B
Tuesday	8:00 AM	316	Synthetic Biology Applications I: Human Health and Disease	MCC	208A
Tuesday	12:30 PM	335	Biosensors, Biodiagnosis and Bioprocess Monitoring I: Synthetic Biology Approach	MCC	206A/B
Tuesday	12:30 PM	362	In silico Systems Biology II: Health Applications	MCC	207A/B

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15C - Bioengineering (continued)					
Tuesday	12:30 PM	390	Synthetic Biology Applications II: Microbial Biosynthesis	MCC	208A
Wednesday	8:00 AM	466	Cell Culture Engineering & Process Design I: Cell Systems Engineering	MCC	208C/D
Wednesday	8:00 AM	504	Protein Engineering I: Therapeutics	MCC	207A/B
Wednesday	8:00 AM	505	Protein Structure, Function, and Stability I: Engineering Technology	MCC	208A
Wednesday	12:30 PM	523	Advances in Protein Expression, Post-Translational Modification and Biomanufacturing	MCC	206A/B
Wednesday	12:30 PM	531	Cell Culture Engineering & Process Design II: Reactor Engineering	MCC	208C/D
Wednesday	12:30 PM	569	Protein Engineering II: Combinatorial Techniques	MCC	207A/B
Wednesday	12:30 PM	570	Protein Structure, Function, and Stability II: Aggregation & Disease	MCC	208A
Wednesday	3:15 PM	626	Protein Engineering III: Rational and Computational Techniques	MCC	207A/B
Wednesday	3:15 PM	627	Protein Structure, Function, and Stability III: Mechanisms	MCC	208A
Thursday	8:00 AM	641	Advances in Biocatalysis and Biosynthesis I: Cellular Engineering Applications	MCC	208C/D
Thursday	8:00 AM	643	Advances in Metabolic Engineering I: Emerging Tools and Techniques	MCC	207A/B
Thursday	8:00 AM	649	Biomolecular Engineering*	MCC	208B
Thursday	8:00 AM	674	Modeling and Engineering Cellular Communities	MCC	208A
Thursday	12:30 PM	692	Advances in Biocatalysis and Biosynthesis II: Enzyme Engineering Applications	MCC	208C/D
Thursday	12:30 PM	693	Advances in Metabolic Engineering II: Value-Added Products from Renewable Feedstocks	MCC	207A/B
Thursday	12:30 PM	697	Bionanotechnology and Micro-Scale Technologies*	MCC	208A
Thursday	12:30 PM	698	Biosensors, Biodiagnosis and Bioprocess Monitoring II: Technology and Device Development	MCC	206A/B
Thursday	3:15 PM	741	Biobased Materials: Design and Application	MCC	103C
Thursday	3:15 PM	752	Industrial Applications of Metabolic Engineering	MCC	103B

15D - Engineering Fundamentals in Life Science					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Sunday	3:30 PM	16	Biomaterials for Nucleic Acid Delivery*	MCC	211C
Sunday	3:30 PM	20	Cells, Organs, and Labs on a Chip	MCC	208B
Sunday	3:30 PM	23	Engineering the Tissue and Cell Microenvironment	MCC	208A
Sunday	3:30 PM	37	Quantitative Approaches to Disease Mechanisms and Therapies I	MCC	207A/B
Monday	8:00 AM	69	Engineering in Cancer Biology and Therapy I	MCC	208B
Monday	12:30 PM	143	Engineering in Cancer Biology and Therapy II	MCC	208B
Monday	12:30 PM	172	Quantitative Approaches to Disease Mechanisms and Therapies II	MCC	208A
Monday	3:15 PM	193	Poster Session: Engineering Fundamentals in Life Science	MCC	Exhibit Hall B
Tuesday	8:00 AM	271	Cell Adhesion and Migration I	MCC	208B
Tuesday	8:00 AM	291	In silico Systems Biology I: Biotechnology Applications*	MCC	207A/B
Tuesday	12:30 PM	339	Cell Adhesion and Migration II	MCC	208B
Tuesday	12:30 PM	362	In silico Systems Biology II: Health Applications*	MCC	207A/B

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15D - Engineering Fundamentals in Life Science (continued)					
Tuesday	3:15 PM	416	Computational Methods in Biological and Biomedical Systems I*	MCC	103F
Wednesday	8:00 AM	476	Drug Delivery I	MCC	208B
Wednesday	8:00 AM	492	Microbial Engineering for Human Health*	MCC	205A/B
Wednesday	12:30 PM	525	Biomaterials for Drug Delivery I: Particle Based Drug Delivery*	MCC	209A/B
Wednesday	12:30 PM	526	Biomaterials for Immunological Applications I: Immune Activation and Vaccination*	MCC	211A
Wednesday	12:30 PM	542	Drug Delivery II	MCC	208B
Wednesday	12:30 PM	566	Probing and Understanding Microbiomes and Microbial Communities*	MCC	205A/B
Wednesday	3:15 PM	590	Applications in Immunology and Immunotherapy	MCC	206A/B
Wednesday	3:15 PM	591	Biomaterials for Drug Delivery II: Micellar, Polymer and Protein Based Drug Carriers*	MCC	211B
Wednesday	3:15 PM	592	Biomaterials for Immunological Applications II: Cancer Immunotherapy and Autoimmune Disease Treatments*	MCC	211A
Wednesday	3:15 PM	598	Drug Delivery III	MCC	208B
Wednesday	3:15 PM	609	Microbial Communities and Microbiomes for Agriculture and Bioenergy*	MCC	205A/B
Wednesday	3:15 PM	630	Stem Cells in Tissue Engineering	MCC	208C/D
Thursday	8:00 AM	647	Biomaterials for Drug Delivery III: Scaffolds Based Drug Delivery*	MCC	210A/B
Thursday	8:00 AM	649	Biomolecular Engineering	MCC	208B
Thursday	8:00 AM	674	Modeling and Engineering Cellular Communities*	MCC	208A
Thursday	12:30 PM	697	Bionanotechnology and Micro-Scale Technologies	MCC	208A
Thursday	12:30 PM	732	Omics and High-Throughput Technologies	MCC	208B
Friday	8:00 AM	770	Biomaterials for in vitro Tissue Models and Improved Therapeutic Strategies*	MCC	102E

16 - Fuels and Petrochemicals Division					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Monday	8:00 AM	64	Division Plenary: Imaging of Heavy Hydrocarbon Molecule Structures	MCC	200A
Monday	12:30 PM	152	In Honor of Stuart W. Churchill I (Invited Talks)*	MCC	101E
Monday	12:30 PM	175	Refinery Distillation	MCC	200A
Monday	12:30 PM	176	Solve this! Fundamental Approach to Problem Solving in Industrial Processes I (Invited Talks)*	MCC	101I
Monday	3:15 PM	228	In Honor of Stuart W. Churchill II (Invited Talks)*	MCC	101E
Monday	3:15 PM	240	Solve this! Fundamental Approach to Problem Solving in Industrial Processes II (Invited Talks)*	MCC	101I
Tuesday	8:00 AM	279	Developments in Petroleum and Biofuels Refining Technologies I	MCC	200A
Tuesday	3:15 PM	417	Conceptual Process Design in Refining, Petrochemicals and Gas Processing	MCC	200A
Wednesday	8:00 AM	484	Future Automotive Catalysis*	MCC	L100D
Wednesday	3:15 PM	584	Poster Session: Fuels and Petrochemicals Division	MCC	Exhibit Hall B

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16D - Alternate Fuels and New Technology					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Monday	3:15 PM	242	Unconventionals: Shale Oil, Oil Sands and Other Heavy Fuels	MCC	200A
Tuesday	12:30 PM	347	Developments in Petroleum and Biofuels Refining Technologies II	MCC	200A
Wednesday	8:00 AM	463	Alternative Fuels and Enabling Technologies	MCC	200A
Wednesday	12:30 PM	578	Unconventionals: Shale Gas, LNG, CNG, and LPG	MCC	200A
Thursday	8:00 AM	690	Unconventionals: Hydrogen and Fuel Cells	MCC	200A
Thursday	12:30 PM	700	Catalytic Biomass Conversion to Chemicals	MCC	200A

17 - Forest and Plant Bioproducts Division					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Sunday	3:30 PM	10	Advances in Algae Based Biorefineries: Algae Biomass Cultivation, Harvesting, and Characterization*	MCC	200D
Monday	8:00 AM	98	Topical Plenary: Advanced Biomaterials, Biofuels, and Biorefinery (Invited Talks)*	MCC	200E
Monday	12:30 PM	129	Biochemical Conversion Processes in Forest/Plant Biomass Biorefineries*	MCC	200E
Monday	12:30 PM	133	Chemical Conversion Processes in Forest/Plant Biorefineries*	MCC	200D
Monday	12:30 PM	152	In Honor of Stuart W. Churchill I (Invited Talks)*	MCC	101E
Monday	12:30 PM	176	Solve this! Fundamental Approach to Problem Solving in Industrial Processes I (Invited Talks)*	MCC	101I
Monday	3:15 PM	202	Poster Session: Novel Products from Forest and Plant Biomass	MCC	Exhibit Hall B
Monday	3:15 PM	228	In Honor of Stuart W. Churchill II (Invited Talks)*	MCC	101E
Monday	3:15 PM	240	Solve this! Fundamental Approach to Problem Solving in Industrial Processes II (Invited Talks)*	MCC	101I
Tuesday	8:00 AM	266	Biomass Characterization, Pretreatment, and Fractionation*	MCC	200E
Tuesday	12:30 PM	386	Separation Processes in Biorefineries*	MCC	200E
Tuesday	3:15 PM	434	Lignin for Sustainable Industrial Uses	MCC	200B
Tuesday	3:15 PM	447	Recalcitrance of Woody Biomass*	MCC	200E
Wednesday	8:00 AM	467	Cellulose-Based Materials	MCC	200E
Wednesday	8:00 AM	490	Lignocellulosic Materials	MCC	200B
Wednesday	12:30 PM	545	Emerging Applications of Cellulose Nanofibrils (CNFs) and Its Composites	MCC	200B
Wednesday	12:30 PM	579	USA-China Progress in Biomass Conversion Technologies I*	MCC	200E
Wednesday	3:15 PM	593	Bioplastics, Biocomposites and Value-Added Uses of Biofuel Coproducts for Sustainable Manufacturing	MCC	200B
Wednesday	3:15 PM	634	USA-China Progress in Biomass Conversion Technologies II*	MCC	200E
Thursday	8:00 AM	652	Chemical Modifications and Processing of Biomaterials	MCC	200D
Thursday	8:00 AM	663	Hydrothermal Carbonization*	MCC	200E
Thursday	12:30 PM	738	Thermochemical Conversion of Biomass*	MCC	200E

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

18 - Liaison Functions

Day	Time	Session #	Session Title	Property	Room
Tuesday	8:00 AM	290	IACChE's James Y. Oldshue Lecture	MCC	Ballroom B

18A - Miscellaneous

Day	Time	Session #	Session Title	Property	Room
Monday	11:00 AM	114	Meet the Executives: Innovating for a Sustainable Future (Invited Talks)	MCC	Ballroom B
Tuesday	12:30 PM	349	Disability Unity Convocation (Invited Talks)	MCC	101H
Tuesday	3:15 PM	398	Poster Session: General Topics on Chemical Engineering I	MCC	Exhibit Hall B
Wednesday	3:15 PM	585	Poster Session: General Topics on Chemical Engineering II	MCC	Exhibit Hall B

18B - Public Affairs and Information Committee (PAIC)

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	8	Public Affairs and AIChE: A PAIC Town Hall	MCC	102A

18C - Young Professionals Committee (YPC)

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	22	Cutting Edge and Innovative Corporate & Industrial Research Projects (Invited Talks)	MCC	101H
Sunday	3:30 PM	25	Green Chemistry and Engineering*	MCC	101D
Sunday	3:30 PM	35	Panel Speakers Forum: Chemical Process and Product Careers in Academia Vs. Industry*	MCC	102B
Sunday	3:30 PM	43	Solids Handling and Processing in the Chemical Industry: What They Don't Teach You at School*	MCC	200J
Sunday	3:30 PM	46	Workshop: Effective Teaching for New or Prospective Faculty*	MCC	205C
Monday	8:00 AM	68	Engineering Government Policy with a Chemical Perspective (Invited Talks)	MCC	101H
Monday	9:30 AM	104	Networking for Nerds: How to Land (or Create) Your Dream Job and Keep Your Career Moving Forward! (Invited Talks)*	MCC	101A
Monday	12:30 PM	128	Biochemical & Biotechnology U.G. Research Session (Invited Talks)	MCC	101H
Monday	12:30 PM	173	Rapid Fire Session: TED-Sep Separations Division*	MCC	M100G
Monday	12:30 PM	176	Solve this! Fundamental Approach to Problem Solving in Industrial Processes I (Invited Talks)	MCC	101I
Monday	12:30 PM	181	Undergraduate Engineering Education of Ethics*	MCC	L100G
Monday	3:15 PM	209	Area Plenary: Sustainability and the RAPID (Rapid Advancement in Process Intensification Deployment) Manufacturing Institute (Invited Talks)*	MCC	101D
Monday	3:15 PM	217	Energy & the Environment U.G. Research Session (Invited Talks)	MCC	101H
Monday	3:15 PM	240	Solve this! Fundamental Approach to Problem Solving in Industrial Processes II (Invited Talks)	MCC	101I
Monday	3:15 PM	243	Use the FE Exam As an Assessment Tool?*	MCC	L100G

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

18C - Young Professionals Committee (YPC) (continued)

Tuesday	8:00 AM	320	Tutorial Session on Electrochemical Methods, Systems and Applications (Invited Talks)*	MCC	M100C
Tuesday	8:00 AM	321	Using the Brains of Others to Innovate Faster*	MCC	L100G
Tuesday	11:00 AM	280	Diversity and Inclusion: Starting and Thriving in the Workplace (Invited Talks)*	MCC	101G
Tuesday	12:30 PM	330	Applied Project Management Fundamentals: A Tutorial*	MCC	L100G
Tuesday	12:30 PM	370	K-12 Outreach Activities and Other Broader Impacts*	MCC	101I
Tuesday	12:30 PM	782	Finding a Healthy Work-Life Balance amid High Stress	MCC	102C
Tuesday	3:15 PM	432	Innovation from Beginning to End: Generating Ideas, Working with People, and Managing Projects*	MCC	L100G
Wednesday	8:00 AM	487	Important Issues in Professional Development Including the Management Division's Award Recipient Presentation (Invited Talks)*	MCC	L100G

18D - Publication Committee

Day	Time	Session #	Session Title	Property	Room
Monday	9:30 AM	104	Networking for Nerds: How to Land (or Create) Your Dream Job and Keep Your Career Moving Forward! (Invited Talks)	MCC	101A
Monday	12:30 PM	116	Poster Presentation Success: How to Prepare and Present a Winning Poster (Invited Talks)	MCC	101A
Monday	1:30 PM	183	Getting Your Research Published (Invited Talks)	MCC	101A

18E - Awards Committee

Day	Time	Session #	Session Title	Property	Room
Tuesday	11:15 AM	325	Andreas Acrivos Award for Professional Progress in Chemical Engineering Lecture	MCC	Ballroom B
Tuesday	6:00 PM	457	SBE's James E. Bailey Award Lecture	MCC	Ballroom B
Wednesday	11:15 AM	517	John M. Prausnitz AIChE Institute Lecture	MCC	Ballroom B

18G - Societal Impact Operating Council (SIOC)

Day	Time	Session #	Session Title	Property	Room
Tuesday	3:15 PM	404	Broadening Participation in Chemical Engineering: Outreach Efforts that Work*	MCC	101I

18I - Minority Affairs Committee (MAC)

Day	Time	Session #	Session Title	Property	Room
Monday	12:30 PM	155	MAC Chemical Engineering Forum (Invited Talks)	MCC	101F
Tuesday	11:00 AM	324	MAC Real Talk: MFF on Academic Career Paths in ChemE (Ticketed Event)	MCC	101F
Tuesday	3:15 PM	404	Broadening Participation in Chemical Engineering: Outreach Efforts that Work*	MCC	101I

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18J - Research and New Technology Committee (RANTC)

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	22	Cutting Edge and Innovative Corporate & Industrial Research Projects (Invited Talks)*	MCC	101H

18L - International Committee

Day	Time	Session #	Session Title	Property	Room
Wednesday	12:30 PM	573	Special Session: Celebrating Prof. Mori's Career Long Accomplishments*	MCC	200I
Wednesday	3:15 PM	607	KIChE-US Chapter Open Forum (Invited Talks)	MCC	102F

18M - Women's Initiatives Committee (WIC)

Day	Time	Session #	Session Title	Property	Room
Sunday	9:00 AM	2	Women Undergraduates Workshop (Ticketed Event)	MCC	101H
Sunday	9:00 AM	3	Women Assistant Professors and Young Scientists: Developing / Your Career (Ticketed Event)	MCC	101G
Sunday	9:00 AM	4	Women Graduate Students and Post-Doctorates Workshop (Ticketed Event)	MCC	101F
Monday	11:00 AM	115	WIC Luncheon (Ticketed Event)	Hilton	Minneapolis Ballroom C
Tuesday	3:15 PM	404	Broadening Participation in Chemical Engineering: Outreach Efforts that Work*	MCC	101I

18N - Assembly of Fellows

Day	Time	Session #	Session Title	Property	Room
Tuesday	3:15 PM	404	Broadening Participation in Chemical Engineering: Outreach Efforts that Work*	MCC	101I

20 - Catalysis and Reaction Engineering Division

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	11	Advances in Industrial Reaction Engineering and Catalysis	MCC	102D
Sunday	3:30 PM	24	Green Chemical Reaction Engineering for Sustainability	MCC	103A
Sunday	3:30 PM	29	Liquid Phase Reaction Engineering	MCC	102E
Sunday	3:30 PM	32	Multi-Scale Modeling	MCC	103B
Sunday	3:30 PM	38	Reaction Engineering of Biomass and Hydrocarbons in Supercritical Water	MCC	102F
Sunday	3:30 PM	41	Science and Engineering of Catalyst Preparation	MCC	103C
Monday	8:00 AM	52	Atomically Dispersed Supported Metal Catalysts I	MCC	L100F
Monday	8:00 AM	58	Catalytic Processing of Fossil and Biorenewable Feedstocks I: Lignin and Bio-Oil Chemistry	MCC	L100C
Monday	8:00 AM	66	Electrocatalysis and Photoelectrocatalysis I: CO_2 Reduction	MCC	L100D
Monday	8:00 AM	77	In Honor of the 2016 Wilhelm Award Winner I (Invited Talks)	MCC	L100A
Monday	8:00 AM	82	Modeling and Analysis of Chemical Reactors	MCC	L100E
Monday	8:00 AM	90	Reactions in Near-Critical and Supercritical Fluids	MCC	L100B
Monday	12:30 PM	121	Applied Environmental Catalysis I	MCC	L100B

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

20 - Catalysis and Reaction Engineering Division (continued)

Monday	12:30 PM	127	Atomically Dispersed Supported Metal Catalysts II	MCC	L100F
Monday	12:30 PM	132	Catalytic Processing of Fossil and Biorenewable Feedstocks II: Carboxylic Acids and Ketones	MCC	L100C
Monday	12:30 PM	141	Electrocatalysis and Photoelectrocatalysis II: HER/HOR	MCC	L100D
Monday	12:30 PM	152	In Honor of Stuart W. Churchill I (Invited Talks)*	MCC	101E
Monday	12:30 PM	153	In Honor of the 2016 Wilhelm Award Winner II (Invited Talks)	MCC	L100A
Monday	12:30 PM	174	Reaction Path Analysis I	MCC	L100E
Monday	12:30 PM	176	Solve this! Fundamental Approach to Problem Solving in Industrial Processes I (Invited Talks)*	MCC	101I
Monday	3:15 PM	207	Applied Environmental Catalysis II	MCC	L100B
Monday	3:15 PM	211	Catalytic Processing of Fossil and Biorenewable Feedstocks III: Alcohols and Polyols	MCC	L100C
Monday	3:15 PM	216	Electrocatalysis and Photoelectrocatalysis III: Computational Methods	MCC	L100D
Monday	3:15 PM	226	In situ and Operando Spectroscopy of Catalysts	MCC	L100F
Monday	3:15 PM	228	In Honor of Stuart W. Churchill II (Invited Talks)*	MCC	101E
Monday	3:15 PM	231	Multiphase Reaction Engineering	MCC	L100A
Monday	3:15 PM	237	Reaction Path Analysis II	MCC	L100E
Monday	3:15 PM	240	Solve this! Fundamental Approach to Problem Solving in Industrial Processes II (Invited Talks)*	MCC	101I
Tuesday	8:00 AM	269	Catalysis with Microporous and Mesoporous Materials I	MCC	L100A
Tuesday	8:00 AM	270	Catalytic Processing of Fossil and Biorenewable Feedstocks IV: Chemistry of Furanics	MCC	L100C
Tuesday	8:00 AM	273	Combustion Kinetics and Emissions I	MCC	L100F
Tuesday	8:00 AM	282	Electrocatalysis and Photoelectrocatalysis IV: ORR/OER	MCC	L100D
Tuesday	8:00 AM	304	New Developments in Computational Catalysis I	MCC	L100E
Tuesday	8:00 AM	308	Reaction Chemistry and Engineering I	MCC	L100B
Tuesday	12:30 PM	336	Breakthroughs in C1 to Chemicals and Processing Engineering*	MCC	103A
Tuesday	12:30 PM	337	Catalysis with Microporous and Mesoporous Materials II	MCC	L100A
Tuesday	12:30 PM	338	Catalytic Processing of Fossil and Biorenewable Feedstocks V: Biomass Deconstruction and Oxygenate Processing	MCC	L100C
Tuesday	12:30 PM	342	Combustion Kinetics and Emissions II	MCC	L100F
Tuesday	12:30 PM	351	Electrocatalysis and Photoelectrocatalysis V: Electrolysis and Solar Fuels	MCC	L100D
Tuesday	12:30 PM	377	New Developments in Computational Catalysis II	MCC	L100E
Tuesday	12:30 PM	385	Reaction Chemistry and Engineering II	MCC	L100B
Tuesday	3:15 PM	405	2017 Practice Award	MCC	L100A
Tuesday	3:15 PM	415	Computational Catalysis I: Fundamentals	MCC	L100E
Tuesday	3:15 PM	422	Electrocatalysis and Photoelectrocatalysis VI: Fuel Oxidation and Chemical Transformations	MCC	L100D
Tuesday	3:15 PM	436	Microreaction Engineering	MCC	L100B
Tuesday	3:15 PM	446	Pyrolysis of Biomass	MCC	L100C
Tuesday	3:15 PM	450	Syngas Production and Gas-to-Liquids Technology	MCC	L100F

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2017 TECHNICAL PROGRAM GRID

20 - Catalysis and Reaction Engineering Division (continued)					
Wednesday	8:00 AM	462	Advances in Process Intensification: Enhanced Reactivity and Separations*	MCC	101E
Wednesday	8:00 AM	465	Catalysis with Microporous and Mesoporous Materials III	MCC	L100A
Wednesday	8:00 AM	469	Computational Catalysis II: Metal and Alloy Catalysis	MCC	L100E
Wednesday	8:00 AM	483	Fundamentals of Surface Reactivity	MCC	L100F
Wednesday	8:00 AM	484	Future Automotive Catalysis	MCC	L100D
Wednesday	8:00 AM	499	Novel Nanoparticles and Nanostructured Materials for Catalysis - Influence of Particle Size*	MCC	200H
Wednesday	8:00 AM	506	Reaction Engineering for Biomass Conversion	MCC	L100C
Wednesday	8:00 AM	507	Reaction Engineering in Pharmaceuticals and Fine Chemicals	MCC	L100B
Wednesday	12:30 PM	528	Catalysis for C1 Chemistry: Producing and Converting Methanol	MCC	L100D
Wednesday	12:30 PM	529	Catalysis for Pharmaceuticals and Fine Chemicals	MCC	L100B
Wednesday	12:30 PM	530	Catalysis with Microporous and Mesoporous Materials IV	MCC	L100A
Wednesday	12:30 PM	533	Chemical and Catalytic Conversions and Processes for Renewable Feedstocks*	MCC	101B
Wednesday	12:30 PM	537	Computational Catalysis III: Electrocatalysis	MCC	L100E
Wednesday	12:30 PM	544	Efficient Processing of Lignin to Bioproducts and Biofuels I*	MCC	103B
Wednesday	12:30 PM	555	Fundamentals of Oxide Catalysis	MCC	L100F
Wednesday	12:30 PM	561	Novel Nanoparticles and Nanostructured Materials for Catalysis - Influence of the Support*	MCC	200H
Wednesday	12:30 PM	571	Reaction Engineering for Combustion and Pyrolysis	MCC	L100C
Wednesday	3:15 PM	582	Poster Session: Catalysis and Reaction Engineering (CRE) Division	MCC	Exhibit Hall B
Wednesday	3:15 PM	608	Membrane Reactors*	MCC	101D
Thursday	8:00 AM	645	Alternative Fuels	MCC	L100C
Thursday	8:00 AM	650	Catalysis for C1 Chemistry: CO_2 Conversion and Methane Reforming	MCC	L100D
Thursday	8:00 AM	651	Catalytic Hydrocarbon Processing I	MCC	L100B
Thursday	8:00 AM	656	Computational Catalysis IV: Biomass Chemistry and Chemicals Production	MCC	L100E
Thursday	8:00 AM	661	Fundamentals of Supported Catalysis I: Hydrocarbon Reactions	MCC	L100F
Thursday	8:00 AM	663	Hydrothermal Carbonization*	MCC	200E
Thursday	8:00 AM	684	Rational Catalyst Design I: Computational Approach	MCC	L100A
Thursday	12:30 PM	699	Catalysis for C1 Chemistry: Methane Reforming and Syngas Conversion	MCC	L100D
Thursday	12:30 PM	701	Catalytic Hydrocarbon Processing II	MCC	L100B
Thursday	12:30 PM	702	Catalytic Hydrogen Generation I: Reforming Reactions	MCC	L100C
Thursday	12:30 PM	703	Computational Catalysis V: Oxides, Zeolites, Porous Catalysts, Etc.	MCC	L100E
Thursday	12:30 PM	715	Fundamentals of Supported Catalysis II: Oxygenate Reactions	MCC	L100F
Thursday	12:30 PM	731	Novel Nanoparticles and Nanostructured Materials for Catalysis - Synthesis and Processing*	MCC	200H
Thursday	12:30 PM	734	Rational Catalyst Design II: Metal Catalysis	MCC	L100A
Thursday	3:15 PM	743	Catalysis for C1 Chemistry: Forming C-C Bonds from Methane	MCC	M100G

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20 - Catalysis and Reaction Engineering Division (continued)					
Thursday	3:15 PM	744	Catalytic Hydrogen Generation II: Shift and Splitting Reactions	MCC	M100E
Thursday	3:15 PM	750	Fundamentals of Supported Catalysis III: Metal/Support Interactions	MCC	M100F
Thursday	3:15 PM	764	Rational Catalyst Design III: Metal Oxide and Compound Catalysis	MCC	M100D
Friday	8:00 AM	779	Reactor Engineering for Biomass Feedstocks*	MCC	101C

21 - Computational Molecular Science and Engineering Forum					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Sunday	8:00 AM	1	Workshop: Hands On With Molecular Simulation (Ticketed Event)	MCC	101I
Sunday	3:30 PM	39	Recent Advances in Molecular Simulation Methods I	MCC	200A
Monday	8:00 AM	70	Faculty Candidates in CoMSEF I: Biomolecules, Soft Materials, and Algorithms	MCC	L100H
Monday	8:00 AM	84	Molecular Simulation of Surface, Interface and Confinement Effects - In Honor of Keith Gubbins' 80th Birthday I (Invited Talks)*	MCC	L100I
Monday	12:30 PM	147	Fundamental, Theory, and Model Development - In Honor of Keith Gubbins' 80th Birthday II (Invited Talks)	MCC	L100H
Monday	12:30 PM	152	In Honor of Stuart W. Churchill I (Invited Talks)*	MCC	101E
Monday	12:30 PM	176	Solve this! Fundamental Approach to Problem Solving in Industrial Processes I (Invited Talks)*	MCC	101I
Monday	3:15 PM	192	Poster Session: Computational Molecular Science and Engineering Forum (CoMSEF)	MCC	Exhibit Hall B
Monday	3:15 PM	218	Faculty Candidates in CoMSEF II: Energy, Catalysis, and Interfaces	MCC	L100H
Monday	3:15 PM	228	In Honor of Stuart W. Churchill II (Invited Talks)*	MCC	101E
Monday	3:15 PM	240	Solve this! Fundamental Approach to Problem Solving in Industrial Processes II (Invited Talks)*	MCC	101I
Tuesday	8:00 AM	260	Applications of Molecular Modeling to Study Interfacial Phenomena	MCC	L100H
Tuesday	8:00 AM	304	New Developments in Computational Catalysis I*	MCC	L100E
Tuesday	12:30 PM	377	New Developments in Computational Catalysis II*	MCC	L100E
Tuesday	12:30 PM	391	The Industrial Fluid Properties Simulation Challenge	MCC	L100H
Tuesday	3:15 PM	415	Computational Catalysis I: Fundamentals*	MCC	L100E
Tuesday	3:15 PM	428	Industrial Applications of Computational Chemistry & Molecular Simulation	MCC	L100H
Wednesday	8:00 AM	469	Computational Catalysis II: Metal and Alloy Catalysis*	MCC	L100E
Wednesday	8:00 AM	508	Recent Advances in Molecular Simulation Methods II	MCC	L100H
Wednesday	12:30 PM	537	Computational Catalysis III: Electrocatalysis*	MCC	L100E
Wednesday	12:30 PM	551	Forum Plenary: Computational Molecular Science and Engineering Forum (Invited Talks)	MCC	L100H
Wednesday	3:15 PM	595	Data Mining and Machine Learning in Molecular Sciences I	MCC	L100H
Wednesday	3:15 PM	614	Molecular Simulation of Adsorption I - In Honor of Keith Gubbins' 80th Birthday III (Invited Talks)*	MCC	M100E
Thursday	8:00 AM	656	Computational Catalysis IV: Biomass Chemistry and Chemicals Production*	MCC	L100E
Thursday	8:00 AM	675	Molecular Modeling of Industrially Relevant Interfacial Phenomena	MCC	L100H
Thursday	8:00 AM	685	Recent Advances in Molecular Simulation III: Free Energy and Phase Equilibrium*	MCC	L100J

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21 - Computational Molecular Science and Engineering Forum (continued)					
Thursday	12:30 PM	703	Computational Catalysis V: Oxides, Zeolites, Porous Catalysts, Etc.*	MCC	L100E
Thursday	12:30 PM	736	Software Engineering in and for the Molecular Sciences	MCC	L100H
Thursday	3:15 PM	747	Data Mining and Machine Learning in Molecular Sciences II	MCC	103A
Friday	8:00 AM	773	Molecular Simulation of Protein Adsorption and Molecular Recognition Processes	MCC	103A

22 - Nanoscale Science and Engineering Forum					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Sunday	3:30 PM	42	Self and Directed Assembly at the Nanoscale	MCC	213A/B
Monday	8:00 AM	62	Division Plenary: Chemical Engineering Principles for Nanotechnology (Invited Talks)	MCC	213A/B
Monday	12:30 PM	152	In Honor of Stuart W. Churchill I (Invited Talks)*	MCC	101E
Monday	12:30 PM	166	Nanomaterials Manufacturing	MCC	212A/B
Monday	12:30 PM	176	Solve this! Fundamental Approach to Problem Solving in Industrial Processes I (Invited Talks)*	MCC	101I
Monday	3:15 PM	201	Poster Session: Nanoscale Science and Engineering	MCC	Exhibit Hall B
Monday	3:15 PM	228	In Honor of Stuart W. Churchill II (Invited Talks)*	MCC	101E
Monday	3:15 PM	240	Solve this! Fundamental Approach to Problem Solving in Industrial Processes II (Invited Talks)*	MCC	101I
Tuesday	8:00 AM	302	Nanoparticles and Health*	MCC	210A/B
Tuesday	12:30 PM	353	Environmental Implications of Nanomaterials: Biological Interactions*	MCC	210A/B
Tuesday	3:15 PM	445	Phase Behavior, Rheology, and Processing of Nanoparticle Suspensions and Solutions	MCC	213A/B
Wednesday	8:00 AM	478	Environmental Applications of Nanotechnology and Nanomaterials I*	MCC	210A/B
Wednesday	3:15 PM	616	Nanofabrication and Nanoscale Processing	MCC	213A/B

22A - Carbon Nanomaterials					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Monday	12:30 PM	131	Carbon Nanomaterials Graduate Student Award Session	MCC	213A/B
Tuesday	8:00 AM	287	Graphene 2-D Materials: Synthesis, Functions and Applications I	MCC	213A/B
Tuesday	12:30 PM	361	Graphene 2-D Materials: Synthesis, Functions and Applications II	MCC	213A/B
Wednesday	8:00 AM	485	Graphene and Carbon Nanotubes: Absorption, Separations, and Transport Processes	MCC	213A/B
Wednesday	12:30 PM	557	Graphene and Carbon Nanotubes: Characterization, Functionalization, and Dispersion	MCC	213A/B
22B - Bionanotechnology					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Sunday	3:30 PM	16	Biomaterials for Nucleic Acid Delivery*	MCC	211C
Sunday	3:30 PM	17	Bionanotechnology for Gene and Drug Delivery I	MCC	212A/B
Monday	8:00 AM	56	Bionanotechnology for Gene and Drug Delivery II	MCC	212A/B

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22B - Bionanotechnology (continued)					
Monday	12:30 PM	128	Biochemical & Biotechnology U.G. Research Session (Invited Talks)*	MCC	101H
Tuesday	8:00 AM	267	Biomaterial Scaffolds for Tissue Engineering I: Anisotropic Materials*	MCC	209A/B
Tuesday	8:00 AM	268	Bionanotechnology Graduate Student Award Session	MCC	212A/B
Tuesday	12:30 PM	331	Area Plenary: Bionanotechnology I (Invited Talks)	MCC	212A/B
Tuesday	12:30 PM	334	Biomaterial Scaffolds for Tissue Engineering II: Bioactive and Drug-Eluting Materials*	MCC	209A/B
Tuesday	12:30 PM	353	Environmental Implications of Nanomaterials: Biological Interactions*	MCC	210A/B
Tuesday	3:15 PM	410	Area Plenary: Bionanotechnology II (Invited Talks)	MCC	212A/B
Wednesday	8:00 AM	496	Nanotechnology for Biotechnology and Pharmaceuticals	MCC	212A/B
Wednesday	12:30 PM	559	Nanobiotechnology for Sensors and Imaging I	MCC	212A/B
Wednesday	3:15 PM	615	Nanobiotechnology for Sensors and Imaging II	MCC	212A/B
Thursday	8:00 AM	676	Nanoscale Science and Engineering in Biomolecular Catalysis I	MCC	212A/B
Thursday	8:00 AM	686	Self-Assembled Biomaterials	MCC	213A/B
Thursday	12:30 PM	727	Nanoscale Science and Engineering in Biomolecular Catalysis II	MCC	212A/B
Thursday	12:30 PM	729	Nanostructured Biomimetic and Biohybrid Materials and Devices	MCC	213A/B

23 - Sustainable Engineering Forum					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Monday	12:30 PM	152	In Honor of Stuart W. Churchill I (Invited Talks)*	MCC	101E
Monday	12:30 PM	176	Solve this! Fundamental Approach to Problem Solving in Industrial Processes I (Invited Talks)*	MCC	101I
Monday	12:30 PM	181	Undergraduate Engineering Education of Ethics*	MCC	L100G
Monday	3:15 PM	222	Fuels from the Sun: Nanomaterials for Water Splitting, Artificial Photosynthesis, and Other Photocatalytic, and Photoelectrochemical Reactions*	MCC	200G
Monday	3:15 PM	228	In Honor of Stuart W. Churchill II (Invited Talks)*	MCC	101E
Monday	3:15 PM	240	Solve this! Fundamental Approach to Problem Solving in Industrial Processes II (Invited Talks)*	MCC	101I
Tuesday	8:00 AM	283	Energy Sustainability: Challenges and Solutions*	MCC	101H
Tuesday	8:00 AM	314	Sustainable Management of Post Consumption/Use Biomaterials*	MCC	101C
Tuesday	8:00 AM	315	Symposium on Solar Power and Chemical Systems in Honor of Prof. Edward A. Fletcher I*	MCC	201A/B
Tuesday	8:00 AM	317	The Energy-Water Nexus*	MCC	102A
Tuesday	12:30 PM	350	Distributed Chemical and Energy Processes for Sustainability*	MCC	101D
Tuesday	12:30 PM	388	Structure in the Design of Sustainable Processes and Supply Chains*	MCC	102A
Tuesday	12:30 PM	389	Symposium on Solar Power and Chemical Systems in Honor of Prof. Edward A. Fletcher II*	MCC	201A/B
Tuesday	3:15 PM	427	CO_2 Industrial, Engineering and R&D Approaches	MCC	102C
Tuesday	3:15 PM	449	Symposium on Solar Power and Chemical Systems in Honor of Prof. Edward A. Fletcher III*	MCC	201A/B
Wednesday	8:00 AM	481	Forum Plenary: Sustainable Engineering Forum (Invited Talks)	MCC	101B

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23 - Sustainable Engineering Forum (continued)					
Wednesday	12:30 PM	528	Catalysis for C1 Chemistry: Producing and Converting Methanol*	MCC	L100D
Wednesday	3:15 PM	587	Poster Session: Sustainability and Sustainable Biorefineries*	MCC	Exhibit Hall B
Thursday	8:00 AM	650	Catalysis for C1 Chemistry: CO_2 Conversion and Methane Reforming*	MCC	L100D
Thursday	8:00 AM	658	Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains I*	MCC	101E
Thursday	12:30 PM	699	Catalysis for C1 Chemistry: Methane Reforming and Syngas Conversion*	MCC	L100D
Thursday	3:15 PM	743	Catalysis for C1 Chemistry: Forming C-C Bonds from Methane*	MCC	M100G

23A - General					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Sunday	3:30 PM	25	Green Chemistry and Engineering	MCC	101D
Monday	8:00 AM	53	Big Data and Sustainability	MCC	101D
Monday	12:30 PM	164	Nanomaterial Applications for Human Health and the Environment	MCC	101D
Monday	12:30 PM	178	The Food-Energy-Water Nexus	MCC	102A
Monday	3:15 PM	209	Area Plenary: Sustainability and the RAPID (Rapid Advancement in Process Intensification Deployment) Manufacturing Institute (Invited Talks)	MCC	101D
Monday	3:15 PM	215	Development of Sustainable New Materials and Intermediates*	MCC	102B
Tuesday	8:00 AM	314	Sustainable Management of Post Consumption/Use Biomaterials	MCC	101C
Tuesday	12:30 PM	387	Separation Process Improvements for Sustainability	MCC	101C
Tuesday	3:15 PM	442	Panel Discussion: Rethinking Grand Challenges in Sustainability for the 21st Century (Invited Talks)	MCC	101C
Wednesday	8:00 AM	481	Forum Plenary: Sustainable Engineering Forum (Invited Talks)*	MCC	101B
Wednesday	12:30 PM	572	Safety and Sustainability Best Practices	MCC	101C
Wednesday	3:15 PM	587	Poster Session: Sustainability and Sustainable Biorefineries	MCC	Exhibit Hall B
Thursday	8:00 AM	681	Process Design: Innovation for Sustainability	MCC	101C

23B - Sustainable Biorefineries					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Sunday	3:30 PM	10	Advances in Algae Based Biorefineries: Algae Biomass Cultivation, Harvesting, and Characterization*	MCC	200D
Sunday	3:30 PM	28	Life Cycle Analysis of Bio-Based Fuels, Energy, and Chemicals	MCC	101B
Monday	8:00 AM	54	Biofuels Production: Design, Simulation, and Economic Analysis	MCC	101B
Monday	8:00 AM	94	Sustainable Energy from Renewable Resources*	MCC	101C
Monday	8:00 AM	98	Topical Plenary: Advanced Biomaterials, Biofuels, and Biorefinery (Invited Talks)*	MCC	200E
Monday	12:30 PM	129	Biochemical Conversion Processes in Forest/Plant Biomass Biorefineries*	MCC	200E
Monday	12:30 PM	133	Chemical Conversion Processes in Forest/Plant Biorefineries*	MCC	200D
Monday	3:15 PM	236	Reaction Kinetics and Transport Fundamentals for Biomass Conversion: Chemical and Catalytic	MCC	101B
Tuesday	8:00 AM	264	Biological Conversions and Processes for Renewable Feedstocks	MCC	101B

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

23B - Sustainable Biorefineries (continued)					
Tuesday	8:00 AM	266	Biomass Characterization, Pretreatment, and Fractionation*	MCC	200E
Tuesday	8:00 AM	307	Process Intensification and Integration of Water and Energy Usage	MCC	101D
Tuesday	12:30 PM	332	Area Plenary: Sustainable Biorefineries (Invited Talks)	MCC	101B
Tuesday	12:30 PM	386	Separation Processes in Biorefineries*	MCC	200E
Tuesday	3:15 PM	420	Distributed Bioprocessing for Integrated Biorefineries	MCC	101D
Tuesday	3:15 PM	447	Recalcitrance of Woody Biomass*	MCC	200E
Tuesday	3:15 PM	455	Value-Added Co-Products from Biorefineries	MCC	101B
Wednesday	8:00 AM	481	Forum Plenary: Sustainable Engineering Forum (Invited Talks)*	MCC	101B
Wednesday	12:30 PM	533	Chemical and Catalytic Conversions and Processes for Renewable Feedstocks	MCC	101B
Wednesday	12:30 PM	544	Efficient Processing of Lignin to Bioproducts and Biofuels I*	MCC	103B
Wednesday	12:30 PM	545	Emerging Applications of Cellulose Nanofibrils (CNFs) and Its Composites*	MCC	200B
Wednesday	12:30 PM	579	USA-China Progress in Biomass Conversion Technologies I*	MCC	200E
Wednesday	3:15 PM	587	Poster Session: Sustainability and Sustainable Biorefineries*	MCC	Exhibit Hall B
Wednesday	3:15 PM	593	Bioplastics, Biocomposites and Value-Added Uses of Biofuel Coproducts for Sustainable Manufacturing*	MCC	200B
Wednesday	3:15 PM	634	USA-China Progress in Biomass Conversion Technologies II*	MCC	200E
Thursday	8:00 AM	659	Developments in Biorefineries	MCC	101B
Thursday	8:00 AM	663	Hydrothermal Carbonization*	MCC	200E
Thursday	8:00 AM	668	Integrated Thermochemical and Biochemical Processing for Renewable Fuels and Chemicals	MCC	101D
Thursday	12:30 PM	695	Biomass Thermal Deconstruction Via Fast Pyrolysis Biorefineries	MCC	101D
Thursday	12:30 PM	714	Feedstock Logistics for Biorefineries	MCC	101B
Thursday	12:30 PM	738	Thermochemical Conversion of Biomass*	MCC	200E
Thursday	3:15 PM	745	Conversion of Biomass Based Renewable Resources to Synthesis Gases and Pyrolysis Oils	MCC	101C
Thursday	3:15 PM	748	Developments in the Pretreatment of Lignocellulosics for Bioconversion	MCC	101A
Thursday	3:15 PM	753	Integrating Municipal and Industrial Waste into Biorefineries	MCC	101B
Friday	8:00 AM	768	Advances in Algal Biorefineries	MCC	101B
Friday	8:00 AM	779	Reactor Engineering for Biomass Feedstocks	MCC	101C

23C - Sustainable Energy					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Sunday	3:30 PM	45	Sustainable Electricity: Generation and Storage	MCC	101C
Monday	8:00 AM	94	Sustainable Energy from Renewable Resources	MCC	101C
Monday	3:15 PM	217	Energy & the Environment U.G. Research Session (Invited Talks)*	MCC	101H
Tuesday	8:00 AM	283	Energy Sustainability: Challenges and Solutions	MCC	101H
Tuesday	8:00 AM	317	The Energy-Water Nexus	MCC	102A
Tuesday	12:30 PM	336	Breakthroughs in C1 to Chemicals and Processing Engineering*	MCC	103A
Tuesday	12:30 PM	350	Distributed Chemical and Energy Processes for Sustainability	MCC	101D

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

23C - Sustainable Energy (continued)					
Wednesday	8:00 AM	481	Forum Plenary: Sustainable Engineering Forum (Invited Talks)*	MCC	101B
Wednesday	3:15 PM	587	Poster Session: Sustainability and Sustainable Biorefineries*	MCC	Exhibit Hall B
Thursday	8:00 AM	658	Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains I	MCC	101E
Thursday	12:30 PM	706	Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains II	MCC	101E

24 - Chemical Engineering & the Law Forum					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Monday	12:30 PM	117	Using Trade Secrets to Protect Chemical Process Innovations	MCC	M100F
Monday	12:30 PM	176	Solve this! Fundamental Approach to Problem Solving in Industrial Processes I (Invited Talks)*	MCC	101I
Monday	1:45 PM	184	How Engineers Can Work Effectively with in-House Counsel	MCC	M100F
Monday	3:15 PM	240	Solve this! Fundamental Approach to Problem Solving in Industrial Processes II (Invited Talks)*	MCC	101I

25 - Upstream Engineering and Flow Assurance Forum					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Monday	8:00 AM	72	Fundamentals and Applications of Flow Assurance	MCC	200B
Monday	12:30 PM	152	In Honor of Stuart W. Churchill I (Invited Talks)*	MCC	101E
Monday	12:30 PM	169	Phase Behavior and Flow of Reservoir Fluids	MCC	200B
Monday	12:30 PM	176	Solve this! Fundamental Approach to Problem Solving in Industrial Processes I (Invited Talks)*	MCC	101I
Monday	3:15 PM	228	In Honor of Stuart W. Churchill II (Invited Talks)*	MCC	101E
Monday	3:15 PM	240	Solve this! Fundamental Approach to Problem Solving in Industrial Processes II (Invited Talks)*	MCC	101I
Tuesday	8:00 AM	286	Gas Hydrates Science and Engineering*	MCC	L100I
Tuesday	8:00 AM	295	Innovations in Production of Unconventional Reservoirs	MCC	200B
Tuesday	12:30 PM	355	Flow Assurance and Asset Integrity	MCC	200B
Tuesday	3:15 PM	403	Poster Session: Upstream Engineering and Flow Assurance	MCC	Exhibit Hall B

26 - Pharmaceutical Discovery, Development and Manufacturing Forum					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Sunday	3:30 PM	14	Amorphous Solid Dispersions for Drug Product	MCC	205A/B
Sunday	3:30 PM	26	Green Pharmaceutical Process Development and Biocatalysis	MCC	204A/B
Monday	8:00 AM	71	Forum Plenary: Pharmaceutical Discovery, Development, and Manufacturing Forum (Invited Talks)	MCC	205A/B
Monday	12:30 PM	136	Computational Solid State Pharmaceutics	MCC	204A/B
Monday	12:30 PM	152	In Honor of Stuart W. Churchill I (Invited Talks)*	MCC	101E
Monday	12:30 PM	162	Model Based Integrated Design of Pharmaceutical Drug Product Processes	MCC	205A/B
Monday	12:30 PM	176	Solve this! Fundamental Approach to Problem Solving in Industrial Processes I (Invited Talks)*	MCC	101I

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26 - Pharmaceutical Discovery, Development and Manufacturing Forum (continued)					
Monday	3:15 PM	203	Poster Session: Pharmaceutical	MCC	Exhibit Hall B
Monday	3:15 PM	228	In Honor of Stuart W. Churchill II (Invited Talks)*	MCC	101E
Monday	3:15 PM	240	Solve this! Fundamental Approach to Problem Solving in Industrial Processes II (Invited Talks)*	MCC	101I
Monday	6:30 PM	251	Pharmaceutical Discovery, Development, and Manufacturing Forum Awards Ceremony	MCC	205A/B
Tuesday	8:00 AM	274	Continuous Processing Technologies Applied in Drug Product Development	MCC	204A/B
Tuesday	8:00 AM	299	Model Based Integrated Design of Pharmaceutical Drug Substance Processes I	MCC	205A/B
Tuesday	8:00 AM	310	Solid Form Selection: Cocrystals, Salts, Solvates, Polymorphs, and Beyond*	MCC	M100J
Tuesday	12:30 PM	344	Continuous Processing Technologies Applied in Drug Product Manufacturing	MCC	204A/B
Tuesday	12:30 PM	373	Model Based Integrated Design of Pharmaceutical Drug Substance Processes II	MCC	205A/B
Tuesday	3:15 PM	418	Continuous Processing Technologies Applied in Drug Substance Development Chemistry	MCC	204A/B
Tuesday	3:15 PM	438	Multivariate Modeling and Quality-by-Control Approaches for Pharmaceutical Processes	MCC	205A/B
Wednesday	8:00 AM	472	Crystallization of Pharmaceutical and Biological Molecules*	MCC	M100J
Wednesday	8:00 AM	500	Panel: Precompetitive Collaboration	MCC	204A/B
Wednesday	8:00 AM	502	Pharmaceutical Process Development and Pilot Plants*	MCC	102C
Wednesday	12:30 PM	539	Continuous Processing Technologies Applied in Drug Substance Development Crystallization and Drying	MCC	204A/B
Wednesday	12:30 PM	541	Diagnostics, Treatments and Theranostics*	MCC	202A/B
Wednesday	12:30 PM	565	PAT for Process Understanding, Reduced Testing, and Elucidation of Fundamental Phenomena in Drug Product/Substance Development	MCC	201A/B
Wednesday	3:15 PM	594	Continuous Processing Technologies Applied in Drug Substance Manufacturing	MCC	204A/B
Wednesday	3:15 PM	596	Development of Processes and Products for Pharmaceuticals and Hybrid Therapeutics	MCC	201A/B
Wednesday	3:15 PM	623	Process Intensification and Advanced Control of Pharmaceutical Processes	MCC	101C
Thursday	8:00 AM	657	Critical Quality Attribute Monitoring and Control in Pharmaceutical Manufacturing I	MCC	205C
Thursday	8:00 AM	665	Innovations in Biopharmaceutical Discovery, Development, and Manufacturing	MCC	204A/B
Thursday	8:00 AM	671	Materials Science in Pharmaceutical Process Development I	MCC	205D
Thursday	12:30 PM	705	Critical Quality Attribute Monitoring and Control in Pharmaceutical Manufacturing II	MCC	205C
Thursday	12:30 PM	717	Innovative Technologies in Pharmaceutical Discovery, Manufacturing and Delivery	MCC	204A/B
Thursday	12:30 PM	720	Materials Science in Pharmaceutical Process Development II	MCC	205D
Thursday	3:15 PM	746	Critical Quality Attribute Monitoring and Control in Pharmaceutical Manufacturing III	MCC	101D

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26 - Pharmaceutical Discovery, Development and Manufacturing Forum (continued)					
Thursday	3:15 PM	762	Quality by Design in Drug Substance Process Development	MCC	101E
Friday	8:00 AM	776	Particle Engineering As Applied to Pharmaceutical Formulations	MCC	101D
Friday	8:00 AM	778	Quality by Design in Drug Product Formulation, Design, and Process Development	MCC	101E

Poster Sessions - Student Chapters Committee Liaison					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Monday	10:00 AM	105	Undergraduate Student Poster Session: Catalysis and Reaction Engineering	MCC	Exhibit Hall B
Monday	10:00 AM	106	Undergraduate Student Poster Session: Computing and Process Control	MCC	Exhibit Hall B
Monday	10:00 AM	107	Undergraduate Student Poster Session: Education & General Papers	MCC	Exhibit Hall B
Monday	10:00 AM	108	Undergraduate Student Poster Session: Environmental	MCC	Exhibit Hall B
Monday	10:00 AM	109	Undergraduate Student Poster Session: Food, Pharmaceutical, and Biotechnology	MCC	Exhibit Hall B
Monday	10:00 AM	110	Undergraduate Student Poster Session: Fuels, Petrochemicals, and Energy	MCC	Exhibit Hall B
Monday	10:00 AM	111	Undergraduate Student Poster Session: Materials Engineering and Sciences	MCC	Exhibit Hall B
Monday	10:00 AM	112	Undergraduate Student Poster Session: Separations	MCC	Exhibit Hall B
Monday	10:00 AM	113	Undergraduate Student Poster Session: Sustainability	MCC	Exhibit Hall B

Poster Sessions					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Sunday	1:00 PM	7	Meet the Faculty Candidate Poster Session*	MCC	Exhibit Hall B
Monday	3:15 PM	186	Interactive Session: Applied Mathematics and Numerical Analysis*	MCC	Exhibit Hall B
Monday	3:15 PM	187	Interactive Session: Data and Information Systems*	MCC	Exhibit Hall B
Monday	3:15 PM	188	Interactive Session: Systems and Process Control*	MCC	Exhibit Hall B
Monday	3:15 PM	189	Interactive Session: Systems and Process Design*	MCC	Exhibit Hall B
Monday	3:15 PM	190	Interactive Session: Systems and Process Operations*	MCC	Exhibit Hall B
Monday	3:15 PM	191	Poster Session: Bioengineering*	MCC	Exhibit Hall B
Monday	3:15 PM	192	Poster Session: Computational Molecular Science and Engineering Forum (CoMSEF)*	MCC	Exhibit Hall B
Monday	3:15 PM	193	Poster Session: Engineering Fundamentals in Life Science*	MCC	Exhibit Hall B
Monday	3:15 PM	194	Poster Session: Food and Bioprocess Engineering*	MCC	Exhibit Hall B
Monday	3:15 PM	195	Poster Session: Interfacial Phenomena (Area 1C)*	MCC	Exhibit Hall B
Monday	3:15 PM	196	Poster Session: Materials Engineering & Sciences (08A - Polymers)*	MCC	Exhibit Hall B
Monday	3:15 PM	197	Poster Session: Materials Engineering & Sciences (08B - Biomaterials)*	MCC	Exhibit Hall B
Monday	3:15 PM	198	Poster Session: Materials Engineering & Sciences (08D - Inorganic Materials)*	MCC	Exhibit Hall B
Monday	3:15 PM	199	Poster Session: Materials Engineering & Sciences (08E - Electronic and Photonic Materials)*	MCC	Exhibit Hall B

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Poster Sessions (continued)					
Monday	3:15 PM	200	Poster Session: Materials Engineering & Sciences (08F - Composite Materials)*	MCC	Exhibit Hall B
Monday	3:15 PM	201	Poster Session: Nanoscale Science and Engineering*	MCC	Exhibit Hall B
Monday	3:15 PM	202	Poster Session: Novel Products from Forest and Plant Biomass*	MCC	Exhibit Hall B
Monday	3:15 PM	203	Poster Session: Pharmaceutical*	MCC	Exhibit Hall B
Monday	3:15 PM	204	Poster Session: Thermodynamics and Transport Properties (Area 1A)*	MCC	Exhibit Hall B
Monday	3:15 PM	234	Poster Session: Fluid Mechanics*	Hilton	Marquette I/II/III/ VIII/IX
Monday	6:00 PM	250	Poster Session: AES*	Hilton	Marquette IV/V/ VI/VII
Tuesday	3:15 PM	396	Poster Session: Chemical Engineering Education*	MCC	Exhibit Hall B
Tuesday	3:15 PM	397	Poster Session: Fundamentals and Applications of Adsorption and Ion Exchange*	MCC	Exhibit Hall B
Tuesday	3:15 PM	399	Poster Session: General Topics on Separations*	MCC	Exhibit Hall B
Tuesday	3:15 PM	400	Poster Session: Particle Technology Forum*	MCC	Exhibit Hall B
Tuesday	3:15 PM	401	Poster Session: Separations Division*	MCC	Exhibit Hall B
Tuesday	3:15 PM	403	Poster Session: Upstream Engineering and Flow Assurance*	MCC	Exhibit Hall B
Wednesday	3:15 PM	582	Poster Session: Catalysis and Reaction Engineering (CRE) Division*	MCC	Exhibit Hall B
Wednesday	3:15 PM	583	Poster Session: Environmental Division*	MCC	Exhibit Hall B
Wednesday	3:15 PM	584	Poster Session: Fuels and Petrochemicals Division*	MCC	Exhibit Hall B
Wednesday	3:15 PM	586	Poster Session: Process Development*	MCC	Exhibit Hall B
Wednesday	3:15 PM	587	Poster Session: Sustainability and Sustainable Biorefineries*	MCC	Exhibit Hall B
Wednesday	6:00 PM	639	Poster Session: Thermal Deconstruction*	MCC	101I

T1 - Meet the Faculty Candidate Poster Session – Sponsored by the Education Division					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Sunday	10:00 AM	5	Workshop: Career Planning for Prospective Faculty*	MCC	101A
Sunday	1:00 PM	7	Meet the Faculty Candidate Poster Session	MCC	Exhibit Hall B
Sunday	3:30 PM	46	Workshop: Effective Teaching for New or Prospective Faculty*	MCC	205C
Monday	8:00 AM	55	Biomaterials: Faculty Candidates*	MCC	211C
Monday	8:00 AM	70	Faculty Candidates in CoMSEF I: Biomolecules, Soft Materials, and Algorithms*	MCC	L100H
Monday	3:15 PM	218	Faculty Candidates in CoMSEF II: Energy, Catalysis, and Interfaces*	MCC	L100H
Tuesday	12:30 PM	352	Electrochemical Fundamentals: Faculty Candidate Session*	MCC	M100C

T3 - 2017 Annual Meeting of the AES Electrophoresis Society					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Monday	9:00 AM	103	Electrokinetics for Cellular Analysis & Separation	Hilton	Marquette IV/V/ VI/VII
Monday	1:15 PM	182	Soft Matter Electrokinetics: Particles, Drops, and Bubbles	Hilton	Marquette IV/V/ VI/VII

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

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T3 - 2017 Annual Meeting of the AES Electrophoresis Society (continued)

Monday	3:30 PM	244	Electrokinetics and Microfluidics for Biomolecular Analysis	Hilton	Marquette IV/V/VI/VII
Monday	6:00 PM	250	Poster Session: AES	Hilton	Marquette IV/V/VI/VII
Tuesday	9:00 AM	323	Electrokinetics for Biological Separation and Analysis	Hilton	Marquette IV/V/VI/VII
Tuesday	1:15 PM	395	Electrokinetics for Sample Preparation	Hilton	Marquette IV/V/VI/VII
Tuesday	3:30 PM	456	Plenary Session: AES Electrophoresis Society (Invited Talks)	Hilton	Marquette IV/V/VI/VII
Wednesday	9:00 AM	516	Electrokinetics: Advancing the Fundamentals	Hilton	Marquette IV/V/VI/VII
Wednesday	1:15 PM	581	Award Session: AES Electrophoresis Society (Invited Talks)	Hilton	Marquette IV/V/VI/VII
Thursday	3:15 PM	749	Directed and Self Assembly of Colloids*	MCC	M100A

T4A - Biorefinery Technologies for Forest Based Lignocellulosic Biomass

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	10	Advances in Algae Based Biorefineries: Algae Biomass Cultivation, Harvesting, and Characterization	MCC	200D
Sunday	3:30 PM	15	Biobased Fuels and Chemicals: Biosynthetic Pathway Engineering & Enzymatic Conversion*	MCC	208C/D
Sunday	3:30 PM	28	Life Cycle Analysis of Bio-Based Fuels, Energy, and Chemicals*	MCC	101B
Sunday	3:30 PM	38	Reaction Engineering of Biomass and Hydrocarbons in Supercritical Water*	MCC	102F
Monday	8:00 AM	54	Biofuels Production: Design, Simulation, and Economic Analysis*	MCC	101B
Monday	8:00 AM	98	Topical Plenary: Advanced Biomaterials, Biofuels, and Biorefinery (Invited Talks)	MCC	200E
Monday	12:30 PM	129	Biochemical Conversion Processes in Forest/Plant Biomass Biorefineries	MCC	200E
Monday	12:30 PM	133	Chemical Conversion Processes in Forest/Plant Biorefineries	MCC	200D
Monday	3:15 PM	202	Poster Session: Novel Products from Forest and Plant Biomass*	MCC	Exhibit Hall B
Monday	3:15 PM	236	Reaction Kinetics and Transport Fundamentals for Biomass Conversion: Chemical and Catalytic*	MCC	101B
Tuesday	8:00 AM	264	Biological Conversions and Processes for Renewable Feedstocks*	MCC	101B
Tuesday	8:00 AM	266	Biomass Characterization, Pretreatment, and Fractionation	MCC	200E
Tuesday	8:00 AM	269	Catalysis with Microporous and Mesoporous Materials I*	MCC	L100A
Tuesday	8:00 AM	307	Process Intensification and Integration of Water and Energy Usage*	MCC	101D
Tuesday	12:30 PM	332	Area Plenary: Sustainable Biorefineries (Invited Talks)*	MCC	101B
Tuesday	12:30 PM	337	Catalysis with Microporous and Mesoporous Materials II*	MCC	L100A
Tuesday	12:30 PM	386	Separation Processes in Biorefineries	MCC	200E
Tuesday	3:15 PM	420	Distributed Bioprocessing for Integrated Biorefineries*	MCC	101D
Tuesday	3:15 PM	434	Lignin for Sustainable Industrial Uses*	MCC	200B
Tuesday	3:15 PM	446	Pyrolysis of Biomass*	MCC	L100C

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

T4A - Biorefinery Technologies for Forest Based Lignocellulosic Biomass (continued)

Tuesday	3:15 PM	447	Recalcitrance of Woody Biomass	MCC	200E
Tuesday	3:15 PM	455	Value-Added Co-Products from Biorefineries*	MCC	101B
Wednesday	8:00 AM	465	Catalysis with Microporous and Mesoporous Materials III*	MCC	L100A
Wednesday	8:00 AM	467	Cellulose-Based Materials*	MCC	200E
Wednesday	8:00 AM	481	Forum Plenary: Sustainable Engineering Forum (Invited Talks)*	MCC	101B
Wednesday	8:00 AM	490	Lignocellulosic Materials*	MCC	200B
Wednesday	8:00 AM	506	Reaction Engineering for Biomass Conversion*	MCC	L100C
Wednesday	12:30 PM	530	Catalysis with Microporous and Mesoporous Materials IV*	MCC	L100A
Wednesday	12:30 PM	533	Chemical and Catalytic Conversions and Processes for Renewable Feedstocks*	MCC	101B
Wednesday	12:30 PM	544	Efficient Processing of Lignin to Bioproducts and Biofuels I*	MCC	103B
Wednesday	12:30 PM	545	Emerging Applications of Cellulose Nanofibrils (CNFs) and Its Composites*	MCC	200B
Wednesday	12:30 PM	579	USA-China Progress in Biomass Conversion Technologies I	MCC	200E
Wednesday	3:15 PM	587	Poster Session: Sustainability and Sustainable Biorefineries*	MCC	Exhibit Hall B
Wednesday	3:15 PM	593	Bioplastics, Biocomposites and Value-Added Uses of Biofuel Coproducts for Sustainable Manufacturing*	MCC	200B
Wednesday	3:15 PM	634	USA-China Progress in Biomass Conversion Technologies II	MCC	200E
Thursday	8:00 AM	652	Chemical Modifications and Processing of Biomaterials*	MCC	200D
Thursday	8:00 AM	659	Developments in Biorefineries*	MCC	101B
Thursday	8:00 AM	663	Hydrothermal Carbonization	MCC	200E
Thursday	8:00 AM	668	Integrated Thermochemical and Biochemical Processing for Renewable Fuels and Chemicals*	MCC	101D
Thursday	12:30 PM	695	Biomass Thermal Deconstruction Via Fast Pyrolysis Biorefineries*	MCC	101D
Thursday	12:30 PM	714	Feedstock Logistics for Biorefineries*	MCC	101B
Thursday	12:30 PM	738	Thermochemical Conversion of Biomass	MCC	200E
Thursday	3:15 PM	745	Conversion of Biomass Based Renewable Resources to Synthesis Gases and Pyrolysis Oils*	MCC	101C
Thursday	3:15 PM	748	Developments in the Pretreatment of Lignocellulosics for Bioconversion*	MCC	101A
Thursday	3:15 PM	753	Integrating Municipal and Industrial Waste into Biorefineries*	MCC	101B
Friday	8:00 AM	768	Advances in Algal Biorefineries*	MCC	101B
Friday	8:00 AM	769	Bio-Based Polymers*	MCC	102A
Friday	8:00 AM	779	Reactor Engineering for Biomass Feedstocks*	MCC	101C

T4B - Symposium on Solar Power and Chemical Systems in Honor of Prof. Edward A. Fletcher

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	45	Sustainable Electricity: Generation and Storage*	MCC	101C
Monday	12:30 PM	156	Materials and Processes for Thermo-, Electro- and Photo-Chemical Energy Storage*	MCC	103B

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

T4B - Symposium on Solar Power and Chemical Systems in Honor of Prof. Edward A. Fletcher (continued)					
Monday	3:15 PM	222	Fuels from the Sun: Nanomaterials for Water Splitting, Artificial Photosynthesis, and Other Photocatalytic, and Photoelectrochemical Reactions*	MCC	200G
Monday	3:15 PM	780	Poster Session: Symposium on Solar Power and Chemical Systems in Honor of Prof. Edward A. Fletcher	MCC	Exhibit Hall B
Tuesday	8:00 AM	315	Symposium on Solar Power and Chemical Systems in Honor of Prof. Edward A. Fletcher I	MCC	201A/B
Tuesday	12:30 PM	389	Symposium on Solar Power and Chemical Systems in Honor of Prof. Edward A. Fletcher II	MCC	201A/B
Tuesday	3:15 PM	449	Symposium on Solar Power and Chemical Systems in Honor of Prof. Edward A. Fletcher III	MCC	201A/B
Friday	8:00 AM	775	Nanostructured/Thin Film Photovoltaics*	MCC	102B

T4C - Hydrogen Production and Storage					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Monday	8:00 AM	48	Advanced Fuel Cell, Hydrogen Generation & Storage Technologies*	MCC	200F
Monday	8:00 AM	78	Materials for Electrochemical Energy I*	MCC	210A/B
Monday	12:30 PM	135	Chemical Looping Processes I*	MCC	103A
Monday	12:30 PM	157	Materials for Electrochemical Energy II*	MCC	210A/B
Monday	3:15 PM	220	Fuel Cell Membranes*	MCC	M100I
Monday	3:15 PM	222	Fuels from the Sun: Nanomaterials for Water Splitting, Artificial Photosynthesis, and Other Photocatalytic, and Photoelectrochemical Reactions*	MCC	200G
Tuesday	8:00 AM	258	Alternative Fuels including Biofuels, Hydrogen, Renewable Hydrogen, and Syngas*	MCC	200F
Tuesday	8:00 AM	301	Nanomaterials for Energy Storage*	MCC	200G
Tuesday	12:30 PM	376	Nanomaterials for Hydrogen Production and Fuel Cells*	MCC	200G
Tuesday	3:15 PM	406	Advances in Catalysis for Hydrogen Production*	MCC	200C
Wednesday	8:00 AM	509	Renewable Hydrogen Production*	MCC	200C
Wednesday	12:30 PM	553	Fuel Processing for Hydrogen Production*	MCC	200C
Wednesday	3:15 PM	622	Polymers for Energy Storage and Conversion*	MCC	211D
Thursday	8:00 AM	690	Unconventionals: Hydrogen and Fuel Cells*	MCC	200A
Thursday	12:30 PM	702	Catalytic Hydrogen Generation I: Reforming Reactions*	MCC	L100C
Thursday	3:15 PM	744	Catalytic Hydrogen Generation II: Shift and Splitting Reactions*	MCC	M100E

T4E - Alternative Energy & Enabling Technologies					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Sunday	3:30 PM	15	Biobased Fuels and Chemicals: Biosynthetic Pathway Engineering & Enzymatic Conversion*	MCC	208C/D
Sunday	3:30 PM	45	Sustainable Electricity: Generation and Storage*	MCC	101C
Monday	8:00 AM	58	Catalytic Processing of Fossil and Biorenewable Feedstocks I: Lignin and Bio-Oil Chemistry*	MCC	L100C

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T4E - Alternative Energy & Enabling Technologies (continued)					
Monday	8:00 AM	66	Electrocatalysis and Photoelectrocatalysis I: CO_2 Reduction*	MCC	L100D
Monday	8:00 AM	94	Sustainable Energy from Renewable Resources*	MCC	101C
Monday	11:00 AM	114	Meet the Executives: Innovating for a Sustainable Future (Invited Talks)*	MCC	Ballroom B
Monday	12:30 PM	132	Catalytic Processing of Fossil and Biorenewable Feedstocks II: Carboxylic Acids and Ketones*	MCC	L100C
Monday	12:30 PM	141	Electrocatalysis and Photoelectrocatalysis II: HER/HOR*	MCC	L100D
Monday	3:15 PM	211	Catalytic Processing of Fossil and Biorenewable Feedstocks III: Alcohols and Polyols*	MCC	L100C
Monday	3:15 PM	216	Electrocatalysis and Photoelectrocatalysis III: Computational Methods*	MCC	L100D
Monday	3:15 PM	224	Fundamentals of Food, Energy, and Water Systems*	MCC	102A
Tuesday	8:00 AM	258	Alternative Fuels including Biofuels, Hydrogen, Renewable Hydrogen, and Syngas*	MCC	200F
Tuesday	8:00 AM	270	Catalytic Processing of Fossil and Biorenewable Feedstocks IV: Chemistry of Furanics*	MCC	L100C
Tuesday	8:00 AM	275	Conversion of Solid Wastes to Energy and/or Product*	MCC	103B
Tuesday	8:00 AM	282	Electrocatalysis and Photoelectrocatalysis IV: ORR/OER*	MCC	L100D
Tuesday	8:00 AM	307	Process Intensification and Integration of Water and Energy Usage*	MCC	101D
Tuesday	12:30 PM	336	Breakthroughs in C1 to Chemicals and Processing Engineering*	MCC	103A
Tuesday	12:30 PM	338	Catalytic Processing of Fossil and Biorenewable Feedstocks V: Biomass Deconstruction and Oxygenate Processing*	MCC	L100C
Tuesday	12:30 PM	350	Distributed Chemical and Energy Processes for Sustainability*	MCC	101D
Tuesday	12:30 PM	351	Electrocatalysis and Photoelectrocatalysis V: Electrolysis and Solar Fuels*	MCC	L100D
Tuesday	3:15 PM	422	Electrocatalysis and Photoelectrocatalysis VI: Fuel Oxidation and Chemical Transformations*	MCC	L100D
Wednesday	8:00 AM	463	Alternative Fuels and Enabling Technologies*	MCC	200A
Wednesday	12:30 PM	538	Conjugated Polymers*	MCC	211C
Wednesday	12:30 PM	544	Efficient Processing of Lignin to Bioproducts and Biofuels I*	MCC	103B
Wednesday	12:30 PM	579	USA-China Progress in Biomass Conversion Technologies I*	MCC	200E
Wednesday	3:15 PM	617	Nanostructured Thin Films*	MCC	209A/B
Wednesday	3:15 PM	622	Polymers for Energy Storage and Conversion*	MCC	211D
Wednesday	3:15 PM	634	USA-China Progress in Biomass Conversion Technologies II*	MCC	200E
Thursday	8:00 AM	645	Alternative Fuels*	MCC	L100C
Thursday	8:00 AM	690	Unconventionals: Hydrogen and Fuel Cells*	MCC	200A
Thursday	12:30 PM	702	Catalytic Hydrogen Generation I: Reforming Reactions*	MCC	L100C
Thursday	12:30 PM	738	Thermochemical Conversion of Biomass*	MCC	200E
Thursday	3:15 PM	744	Catalytic Hydrogen Generation II: Shift and Splitting Reactions*	MCC	M100E
Friday	8:00 AM	775	Nanostructured/Thin Film Photovoltaics*	MCC	102B
Friday	8:00 AM	779	Reactor Engineering for Biomass Feedstocks*	MCC	101C

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T4F - BioFuels

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	10	Advances in Algae Based Biorefineries: Algae Biomass Cultivation, Harvesting, and Characterization*	MCC	200D
Sunday	3:30 PM	15	Biobased Fuels and Chemicals: Biosynthetic Pathway Engineering & Enzymatic Conversion*	MCC	208C/D
Monday	8:00 AM	58	Catalytic Processing of Fossil and Biorenewable Feedstocks I: Lignin and Bio-Oil Chemistry*	MCC	L100C
Monday	8:00 AM	95	Sustainable Microbial Process for Food, Feeds, Energy, and Environment*	MCC	103B
Monday	8:00 AM	98	Topical Plenary: Advanced Biomaterials, Biofuels, and Biorefinery (Invited Talks)*	MCC	200E
Monday	12:30 PM	129	Biochemical Conversion Processes in Forest/Plant Biomass Biorefineries*	MCC	200E
Monday	12:30 PM	132	Catalytic Processing of Fossil and Biorenewable Feedstocks II: Carboxylic Acids and Ketones*	MCC	L100C
Monday	12:30 PM	133	Chemical Conversion Processes in Forest/Plant Biorefineries*	MCC	200D
Monday	3:15 PM	211	Catalytic Processing of Fossil and Biorenewable Feedstocks III: Alcohols and Polyols*	MCC	L100C
Tuesday	8:00 AM	258	Alternative Fuels including Biofuels, Hydrogen, Renewable Hydrogen, and Syngas*	MCC	200F
Tuesday	8:00 AM	266	Biomass Characterization, Pretreatment, and Fractionation*	MCC	200E
Tuesday	8:00 AM	270	Catalytic Processing of Fossil and Biorenewable Feedstocks IV: Chemistry of Furanics*	MCC	L100C
Tuesday	8:00 AM	275	Conversion of Solid Wastes to Energy and/or Product*	MCC	103B
Tuesday	8:00 AM	279	Developments in Petroleum and Biofuels Refining Technologies I*	MCC	200A
Tuesday	12:30 PM	338	Catalytic Processing of Fossil and Biorenewable Feedstocks V: Biomass Deconstruction and Oxygenate Processing*	MCC	L100C
Tuesday	12:30 PM	347	Developments in Petroleum and Biofuels Refining Technologies II*	MCC	200A
Wednesday	12:30 PM	544	Efficient Processing of Lignin to Bioproducts and Biofuels I*	MCC	103B
Wednesday	12:30 PM	579	USA-China Progress in Biomass Conversion Technologies I*	MCC	200E
Wednesday	3:15 PM	600	Efficient Processing of Lignin to Bioproducts and Biofuels II*	MCC	103B
Wednesday	3:15 PM	634	USA-China Progress in Biomass Conversion Technologies II*	MCC	200E
Thursday	8:00 AM	656	Computational Catalysis IV: Biomass Chemistry and Chemicals Production*	MCC	L100E
Thursday	8:00 AM	676	Nanoscale Science and Engineering in Biomolecular Catalysis I*	MCC	212A/B
Thursday	8:00 AM	690	Unconventionals: Hydrogen and Fuel Cells*	MCC	200A
Thursday	12:30 PM	722	Membrane Formation*	MCC	M100I
Thursday	12:30 PM	738	Thermochemical Conversion of Biomass*	MCC	200E

T4G - Fossil Fuels & CCS

Day	Time	Session #	Session Title	Property	Room
Monday	8:00 AM	57	Carbon Dioxide Capture from Power Generation*	MCC	200C
Monday	12:30 PM	121	Applied Environmental Catalysis I*	MCC	L100B
Monday	12:30 PM	135	Chemical Looping Processes I*	MCC	103A

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T4G - Fossil Fuels & CCS (continued)

Monday	12:30 PM	138	CO_2 Use and Reuse*	MCC	200C
Monday	3:15 PM	207	Applied Environmental Catalysis II*	MCC	L100B
Monday	3:15 PM	232	Novel Approaches to CO2 Utilization*	MCC	200C
Tuesday	8:00 AM	269	Catalysis with Microporous and Mesoporous Materials I*	MCC	L100A
Tuesday	8:00 AM	273	Combustion Kinetics and Emissions I*	MCC	L100F
Tuesday	8:00 AM	276	CO_2 Capture By Adsorption I: Process and Storage*	MCC	M100F
Tuesday	8:00 AM	317	The Energy-Water Nexus*	MCC	102A
Tuesday	8:00 AM	322	Value-Added Chemicals from Natural Gas*	MCC	200C
Tuesday	12:30 PM	337	Catalysis with Microporous and Mesoporous Materials II*	MCC	L100A
Tuesday	12:30 PM	342	Combustion Kinetics and Emissions II*	MCC	L100F
Tuesday	12:30 PM	346	CO_2 Capture, Utilization, and Disposal: Key to Clean Energy Production I*	MCC	200F
Tuesday	3:15 PM	412	Carbon Dioxide Capture Technologies and Their Use*	MCC	102F
Tuesday	3:15 PM	454	Unconventional Technologies for CO_2 Capture, Conversion and Utilization*	MCC	103B
Wednesday	8:00 AM	465	Catalysis with Microporous and Mesoporous Materials III*	MCC	L100A
Wednesday	8:00 AM	471	CO_2 Capture, Utilization, and Disposal: Key to Clean Energy Production II*	MCC	200F
Wednesday	8:00 AM	484	Future Automotive Catalysis*	MCC	L100D
Wednesday	8:00 AM	513	Topical Plenary: Chemical Engineers in Medicine III (Invited Talks)*	MCC	202A/B
Wednesday	12:30 PM	530	Catalysis with Microporous and Mesoporous Materials IV*	MCC	L100A
Wednesday	12:30 PM	534	Coal Conversion to Value-Added Chemicals and Power in Modular Systems*	MCC	101D
Wednesday	12:30 PM	558	Modeling and Computation in Energy and Environment*	MCC	103F
Wednesday	12:30 PM	571	Reaction Engineering for Combustion and Pyrolysis*	MCC	L100C
Wednesday	3:15 PM	589	Advances in Unconventional Oil and Gas Modeling*	MCC	200C
Thursday	8:00 AM	650	Catalysis for C1 Chemistry: CO_2 Conversion and Methane Reforming*	MCC	L100D
Thursday	8:00 AM	672	Membranes for CO_2 Separations - GS IV*	MCC	M100I
Thursday	8:00 AM	678	Novel Materials and Processes for Air Pollution Control*	MCC	103B
Thursday	12:30 PM	707	Design and Optimization of Environmentally Sustainable Advanced Fossil Energy Systems*	MCC	200C
Thursday	3:15 PM	763	Rare Earth Elements in Fossil Fuel Derived Solids and Liquids*	MCC	200C
Friday	8:00 AM	772	Engineering Geologic Carbon Dioxide Storage Systems*	MCC	101A

T4H – 2017 International Congress on Energy (ICE)

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	8	Public Affairs and AIChE: A PAIC Town Hall*	MCC	102A
Monday	8:00 AM	57	Carbon Dioxide Capture from Power Generation*	MCC	200C
Monday	8:00 AM	68	Engineering Government Policy with a Chemical Perspective (Invited Talks)*	MCC	101H
Monday	8:00 AM	100	World Café: Food-Energy-Water Nexus (Invited Talks)*	MCC	102A
Monday	12:30 PM	178	The Food-Energy-Water Nexus*	MCC	102A

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T4H – 2017 International Congress on Energy (ICE) (continued)					
Tuesday	8:00 AM	317	The Energy-Water Nexus*	MCC	102A
Tuesday	12:30 PM	394	Topical Plenary: Advances in Fossil Energy R&D (Invited Talks)*	MCC	200C
Tuesday	3:15 PM	451	Nexus Forum - Options for Addressing Complex, Interconnected Systems*	MCC	102A
Wednesday	12:30 PM	534	Coal Conversion to Value-Added Chemicals and Power in Modular Systems*	MCC	101D

T5 - Nanomaterials for Applications in Energy and Biology					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Monday	8:00 AM	85	Nanomaterials for Biological Applications I	MCC	200G
Monday	12:30 PM	165	Nanomaterials for Biological Applications II	MCC	200G
Monday	3:15 PM	222	Fuels from the Sun: Nanomaterials for Water Splitting, Artificial Photosynthesis, and Other Photocatalytic, and Photoelectrochemical Reactions	MCC	200G
Tuesday	8:00 AM	301	Nanomaterials for Energy Storage	MCC	200G
Tuesday	12:30 PM	353	Environmental Implications of Nanomaterials: Biological Interactions*	MCC	210A/B
Tuesday	12:30 PM	376	Nanomaterials for Hydrogen Production and Fuel Cells	MCC	200G
Tuesday	3:15 PM	440	Nanomaterials for Light Harvesting and Novel Photophysical Phenomenon I	MCC	200G
Wednesday	8:00 AM	478	Environmental Applications of Nanotechnology and Nanomaterials I*	MCC	210A/B
Wednesday	8:00 AM	495	Nanomaterials for Light Harvesting and Novel Photophysical Phenomenon II	MCC	200G
Thursday	12:30 PM	735	Semiconducting Quantum Dots I: Surface Chemistry and Assemblies*	MCC	210A/B
Thursday	3:15 PM	765	Semiconducting Quantum Dots II: Novel Syntheses and Devices*	MCC	102B

T6 - Next-Gen Manufacturing					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Sunday	3:30 PM	22	Cutting Edge and Innovative Corporate & Industrial Research Projects (Invited Talks)*	MCC	101H
Monday	8:00 AM	89	Rapid Process Intensification Institute Update*	MCC	101E
Monday	11:00 AM	114	Meet the Executives: Innovating for a Sustainable Future (Invited Talks)*	MCC	Ballroom B
Tuesday	12:30 PM	155	MAC Chemical Engineering Forum (Invited Talks)*	MCC	101F
Monday	3:15 PM	209	Area Plenary: Sustainability and the RAPID (Rapid Advancement in Process Intensification Deployment) Manufacturing Institute (Invited Talks)*	MCC	101D
Tuesday	8:00 AM	252	3D Printing Fundamentals and Applications	MCC	101A
Tuesday	8:00 AM	257	Advances in Process Intensification: Enhanced Mass Transfer*	MCC	101E
Tuesday	8:00 AM	307	Process Intensification and Integration of Water and Energy Usage*	MCC	101D
Tuesday	12:30 PM	344	Continuous Processing Technologies Applied in Drug Product Manufacturing*	MCC	204A/B
Tuesday	12:30 PM	350	Distributed Chemical and Energy Processes for Sustainability*	MCC	101D
Tuesday	12:30 PM	382	Process Intensification By Process Integration*	MCC	101E

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T6 - Next-Gen Manufacturing (continued)					
Tuesday	3:15 PM	408	Advances in Process Intensification*	MCC	101E
Tuesday	3:15 PM	418	Continuous Processing Technologies Applied in Drug Substance Development Chemistry*	MCC	204A/B
Tuesday	3:15 PM	420	Distributed Bioprocessing for Integrated Biorefineries*	MCC	101D
Tuesday	3:15 PM	781	Smart Manufacturing – the Clean Energy Smart Manufacturing Innovation Institute	MCC	101A
Wednesday	8:00 AM	462	Advances in Process Intensification: Enhanced Reactivity and Separations*	MCC	101E
Wednesday	8:00 AM	503	Process Intensification through Process Systems Engineering*	MCC	101D
Wednesday	11:15 AM	517	John M. Prausnitz AIChE Institute Lecture*	MCC	Ballroom B
Wednesday	12:30 PM	534	Coal Conversion to Value-Added Chemicals and Power in Modular Systems*	MCC	101D
Wednesday	12:30 PM	567	Process Intensification through the Application of Microreactors and Membrane Reactors*	MCC	101E
Wednesday	3:15 PM	594	Continuous Processing Technologies Applied in Drug Substance Manufacturing*	MCC	204A/B
Wednesday	3:15 PM	608	Membrane Reactors*	MCC	101D
Wednesday	3:15 PM	623	Process Intensification and Advanced Control of Pharmaceutical Processes*	MCC	101C
Wednesday	3:15 PM	624	Process Intensification By Enhanced Heat and Mass Transfer*	MCC	101E
Thursday	8:00 AM	648	Biomaterials I: Instructive and Responsive Biomaterials*	MCC	211A
Thursday	12:30 PM	717	Innovative Technologies in Pharmaceutical Discovery, Manufacturing and Delivery*	MCC	204A/B
Friday	8:00 AM	777	Polymers in Additive Manufacturing*	MCC	102D

T7 - The Food-Energy-Water Nexus					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Sunday	3:30 PM	8	Public Affairs and AIChE: A PAIC Town Hall*	MCC	102A
Monday	8:00 AM	68	Engineering Government Policy with a Chemical Perspective (Invited Talks)*	MCC	101H
Monday	8:00 AM	100	World Café: Food-Energy-Water Nexus (Invited Talks)	MCC	102A
Monday	12:30 PM	178	The Food-Energy-Water Nexus*	MCC	102A
Monday	12:30 PM	181	Undergraduate Engineering Education of Ethics*	MCC	L100G
Monday	3:15 PM	209	Area Plenary: Sustainability and the RAPID (Rapid Advancement in Process Intensification Deployment) Manufacturing Institute (Invited Talks)*	MCC	101D
Monday	3:15 PM	224	Fundamentals of Food, Energy, and Water Systems*	MCC	102A
Tuesday	8:00 AM	317	The Energy-Water Nexus*	MCC	102A
Tuesday	12:30 PM	388	Structure in the Design of Sustainable Processes and Supply Chains*	MCC	102A
Tuesday	3:15 PM	451	Nexus Forum - Options for Addressing Complex, Interconnected Systems	MCC	102A

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T8 - Process Intensification & Modular Chemical Processing

Day	Time	Session #	Session Title	Property	Room
Monday	8:00 AM	89	RAPID Process Intensification Institute Update	MCC	101E
Monday	3:15 PM	209	Area Plenary: Sustainability and the RAPID (Rapid Advancement in Process Intensification Deployment) Manufacturing Institute (Invited Talks)*	MCC	101D
Tuesday	8:00 AM	257	Advances in Process Intensification: Enhanced Mass Transfer	MCC	101E
Tuesday	8:00 AM	307	Process Intensification and Integration of Water and Energy Usage*	MCC	101D
Tuesday	12:30 PM	350	Distributed Chemical and Energy Processes for Sustainability*	MCC	101D
Tuesday	12:30 PM	382	Process Intensification By Process Integration*	MCC	101E
Tuesday	3:15 PM	408	Advances in Process Intensification*	MCC	101E
Tuesday	3:15 PM	420	Distributed Bioprocessing for Integrated Biorefineries*	MCC	101D
Wednesday	8:00 AM	462	Advances in Process Intensification: Enhanced Reactivity and Separations	MCC	101E
Wednesday	8:00 AM	503	Process Intensification through Process Systems Engineering*	MCC	101D
Wednesday	12:30 PM	534	Coal Conversion to Value-Added Chemicals and Power in Modular Systems*	MCC	101D
Wednesday	12:30 PM	567	Process Intensification through the Application of Microreactors and Membrane Reactors*	MCC	101E
Wednesday	3:15 PM	608	Membrane Reactors*	MCC	101D
Wednesday	3:15 PM	623	Process Intensification and Advanced Control of Pharmaceutical Processes*	MCC	101C
Wednesday	3:15 PM	624	Process Intensification By Enhanced Heat and Mass Transfer*	MCC	101E

T9 - Sensors

Day	Time	Session #	Session Title	Property	Room
Monday	12:30 PM	130	Biosensor Devices: Applications	MCC	M100A
Monday	3:15 PM	241	Topical Plenary: Advances in Biosensing (Invited Talks)	MCC	M100A
Tuesday	8:00 AM	297	Materials Chemistry for Biosensors	MCC	M100A
Tuesday	12:30 PM	372	Micro and Nanofabricated Sensors	MCC	M100A

TA - Microbiomes and Microbial Communities

Day	Time	Session #	Session Title	Property	Room
Wednesday	8:00 AM	492	Microbial Engineering for Human Health	MCC	205A/B
Wednesday	12:30 PM	566	Probing and Understanding Microbiomes and Microbial Communities	MCC	205A/B
Wednesday	3:15 PM	609	Microbial Communities and Microbiomes for Agriculture and Bioenergy	MCC	205A/B

TB - Thermal Deconstruction of Biomass

Day	Time	Session #	Session Title	Property	Room
Wednesday	8:00 AM	501	Pathways to Thermal Deconstruction	MCC	101I
Wednesday	12:30 PM	556	Fundamentals of Thermal Deconstruction	MCC	101I
Wednesday	3:15 PM	633	Upgrading Products of Thermal Deconstruction	MCC	101I
Wednesday	6:00 PM	639	Poster Session: Thermal Deconstruction	MCC	101I

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

Day	Time	Session #	Session Title	Property	Room
Tuesday	8:00 AM	302	Nanoparticles and Health	MCC	210A/B
Tuesday	12:30 PM	353	Environmental Implications of Nanomaterials: Biological Interactions	MCC	210A/B
Wednesday	8:00 AM	478	Environmental Applications of Nanotechnology and Nanomaterials I	MCC	210A/B
Wednesday	12:30 PM	549	Environmental Applications of Nanotechnology and Nanomaterials II	MCC	210A/B

TD - NH_3 Energy$^+$ - Enabling Optimized, Sustainable Energy and Agriculture

Day	Time	Session #	Session Title	Property	Room
Wednesday	8:00 AM	498	NH_3 Energy Overview and Safety	MCC	101F/G
Wednesday	12:30 PM	560	NH_3 Fuel End Use	MCC	101F/G
Wednesday	3:15 PM	618	NH_3 Fuel End Use and Synthesis	MCC	101F/G
Wednesday	6:00 PM	638	Poster Session: NH_3 Energy$^+$	MCC	101F/G
Thursday	8:00 AM	677	NH_3 Fuel Synthesis I	MCC	101F/G
Thursday	12:30 PM	730	NH_3 Fuel Synthesis II	MCC	101F/G

TE - Advances in Fossil Energy R&D

Day	Time	Session #	Session Title	Property	Room
Monday	8:00 AM	57	Carbon Dioxide Capture from Power Generation	MCC	200C
Monday	12:30 PM	138	CO_2 Use and Reuse	MCC	200C
Monday	3:15 PM	232	Novel Approaches to CO_2 Utilization	MCC	200C
Tuesday	8:00 AM	273	Combustion Kinetics and Emissions I*	MCC	L100F
Tuesday	8:00 AM	322	Value-Added Chemicals from Natural Gas	MCC	200C
Tuesday	12:30 PM	336	Breakthroughs in C1 to Chemicals and Processing Engineering*	MCC	103A
Tuesday	12:30 PM	342	Combustion Kinetics and Emissions II*	MCC	L100F
Tuesday	12:30 PM	394	Topical Plenary: Advances in Fossil Energy R&D (Invited Talks)	MCC	200C
Tuesday	3:15 PM	406	Advances in Catalysis for Hydrogen Production	MCC	200C
Wednesday	8:00 AM	509	Renewable Hydrogen Production	MCC	200C
Wednesday	12:30 PM	534	Coal Conversion to Value-Added Chemicals and Power in Modular Systems	MCC	101D
Wednesday	12:30 PM	553	Fuel Processing for Hydrogen Production	MCC	200C
Wednesday	12:30 PM	571	Reaction Engineering for Combustion and Pyrolysis*	MCC	L100C
Wednesday	3:15 PM	589	Advances in Unconventional Oil and Gas Modeling	MCC	200C
Thursday	8:00 AM	644	Advances in Shale Characterization and Fluids Management	MCC	200C
Thursday	12:30 PM	707	Design and Optimization of Environmentally Sustainable Advanced Fossil Energy Systems	MCC	200C
Thursday	3:15 PM	763	Rare Earth Elements in Fossil Fuel Derived Solids and Liquids	MCC	200C
Friday	8:00 AM	772	Engineering Geologic Carbon Dioxide Storage Systems	MCC	101A

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TF - Chemical Engineers in Medicine					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Monday	8:00 AM	99	Topical Plenary: Chemical Engineers in Medicine I (Invited Talks)	MCC	202A/B
Monday	12:30 PM	134	Chemical Engineering Principles Advancing Medicine I	MCC	202A/B
Monday	3:15 PM	229	Medical Devices	MCC	202A/B
Tuesday	8:00 AM	319	Topical Plenary: Chemical Engineers in Medicine II (Invited Talks)	MCC	202A/B
Tuesday	12:30 PM	340	Chemical Engineering Principles Advancing Medicine II	MCC	202A/B
Wednesday	8:00 AM	513	Topical Plenary: Chemical Engineers in Medicine III (Invited Talks)	MCC	202A/B
Wednesday	12:30 PM	541	Diagnostics, Treatments and Theranostics	MCC	202A/B

TG - Innovations of Green Process Engineering for Sustainable Energy and Environment					
Day	**Time**	**Session #**	**Session Title**	**Property**	**Room**
Sunday	3:30 PM	24	Green Chemical Reaction Engineering for Sustainability*	MCC	103A
Sunday	3:30 PM	28	Life Cycle Analysis of Bio-Based Fuels, Energy, and Chemicals*	MCC	101B
Monday	8:00 AM	86	Novel Catalytic and Separation Process Based on Ionic Liquids	MCC	103A
Monday	8:00 AM	95	Sustainable Microbial Process for Food, Feeds, Energy, and Environment	MCC	103B
Monday	12:30 PM	135	Chemical Looping Processes I	MCC	103A
Monday	12:30 PM	156	Materials and Processes for Thermo-, Electro- and Photo-Chemical Energy Storage	MCC	103B
Monday	3:15 PM	212	Chemical Looping Processes II	MCC	103A
Monday	3:15 PM	215	Development of Sustainable New Materials and Intermediates*	MCC	102B
Monday	3:15 PM	217	Energy & the Environment U.G. Research Session (Invited Talks)*	MCC	101H
Monday	3:15 PM	238	Research Frontier of Water Sustainability	MCC	103B
Tuesday	8:00 AM	275	Conversion of Solid Wastes to Energy and/or Product	MCC	103B
Tuesday	8:00 AM	318	Topical Plenary: Award Speaker Session for Green Process Engineering (Invited Talks)	MCC	103A
Tuesday	12:30 PM	336	Breakthroughs in C1 to Chemicals and Processing Engineering	MCC	103A
Tuesday	12:30 PM	368	Integrated Process Engineering and Economics Analysis	MCC	103B
Tuesday	3:15 PM	437	Modeling & Simulation of Complex Systems	MCC	103A
Tuesday	3:15 PM	454	Unconventional Technologies for CO_2 Capture, Conversion and Utilization	MCC	103B
Tuesday	3:15 PM	455	Value-Added Co-Products from Biorefineries*	MCC	101B
Wednesday	8:00 AM	489	Ionic Liquids: Thermodynamics and Properties	MCC	103B
Wednesday	12:30 PM	544	Efficient Processing of Lignin to Bioproducts and Biofuels I	MCC	103B
Wednesday	3:15 PM	600	Efficient Processing of Lignin to Bioproducts and Biofuels II	MCC	103B
Thursday	8:00 AM	658	Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains I*	MCC	101E
Thursday	8:00 AM	678	Novel Materials and Processes for Air Pollution Control	MCC	103B
Thursday	12:30 PM	714	Feedstock Logistics for Biorefineries*	MCC	101B

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

SPONSORED TECHNOLOGY WORKSHOPS

Learn about the latest technologies that can help your research at Sponsored Technology Workshops. Companies will provide you with an opportunity to see the most cutting edge developments in chemical engineering technology that can help you in your current and future positions.

LOCATION: MINNEAPOLIS CONVENTION CENTER, 101J

ANSYS

ANSYS: Simulation and Analysis Software for Chemical and Process Engineering
Monday, October 30 • 3:15 PM - 4:30 PM

Engineering problems and projects are now cross functional and multi-disciplinary. The industry investments are increasingly more complex driven by for requirements for sustainability, energy efficiency, higher performance, and global competition. Built on a set of well-establish physics based modeling and computational techniques engineering simulation has moved from R&D center use to a broader enterprise deployment.

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

Chemstations™

Chemstations: Integrating Global Simulation Competition into Senior Design
Monday, October 30 • 12:30 PM - 1:15 PM
Tuesday, October 31 • 8:00 AM - 8:45 AM and 12:30 PM - 1:15 PM

University of New Hampshire Assistant Professor, Jeffrey Halpern, engaged his students in the 2017 Process Simulation Cup as part of their design course. Dr. Halpern will join Chemstations at this workshop to share learnings from this experience. The Process Simulation Cup is a global competition to optimize a given flowsheet representing a typical optimization problem. The Process Simulation Cup is open to university students, providing a way for them to both test and demonstrate advanced use of a process simulator. Learn more about the Process Simulation Cup below or at https://www.process-simulation-cup.com/about-cup/.

The Process Simulation Cup is a unique chance for chemical engineering students to learn about process simulation and to gain valuable industry exposure. The task is to optimize a given flowsheet representing a typical optimization problem of the chemical, pharmaceutical or life science industries. The challenge problem is believed to have several local optima and a global optimum, but no closed solution. Finding an optimum requires tenacity and ingenuity - both are desirable professional skills for an excellent engineer. Awards are presented for the participant & institution who has submitted the best design variables. In February 2018, the 2017 Process Simulation Cup champion will be announced. The Process Simulation Cup is organized by Chemstations Europe GmbH, Berlin.

IndianOil

Indian Oil Corporation:
Overview of Indian Oil R&D — Technology Basket Value Creation through Technology Selection: Indian Oil Offerings
Wednesday, November 1 • 8:00 AM - 10:30 AM

PSE

Process Systems Enterprise:
Hands-On Workshop: Mechanistic Models For The Digital Design Of Robust Formulated Products and Their Manufacturing Processes
Tuesday, October 31 • 3:15 PM - 5:45 PM

Join PSE and industry experts for a hands-on software demonstration of the newly released gPROMS Formulated Products, an innovative platform for the digital design of formulated products and their manufacturing processes. Currently, scientists and engineers in the pharmaceutical, biopharmaceutical, food and consumer goods industries face enormous challenges in efficiently bringing products to market with robust manufacturing processes to produce the desired end-use attributes. Historically, upstream process design choices and formulation decisions have been very difficult to tie to final product characteristics.

gPROMS Formulated Products allows scientists and engineers to screen formulations for end-user attributes, determine whether they can be manufactured efficiently and robustly, and explore the design space of the whole formulation and manufacturing chain.

Quantachrome INSTRUMENTS

Quantachrome Instruments
Progress and Challenges in the Structural Characterization of Nanoporous Materials by Physical Adsorption
Thursday, November 2 • 10:30 AM - 11:00 AM

We will discuss important fundamental aspects of the underlying adsorption mechanisms of fluids and nanoporous materials (e.g., micro-mesoporous materials with hierarchical pore structure [4]) and their significance for physical adsorption characterization.

[4] K. A. Cychosz, R. Guillet-Nicolas, J. Garcia-Martinez, J., M. Thommes, M. Chem. Soc. Rev. 46, 389, (2017)

High Pressure Adsorption Techniques for Assessing Adsorbents for Capture and Storage Applications
Thursday, November 2 • 11:00 AM - 11:30 AM

Use of porous materials for the capture and storage of gasses has been of interest for many years. We will discuss the use of a commercially available high pressure gas sorption apparatus for the characterization of materials for gas capture and storage.

Use of Dynamic Breakthrough Measurements for Characterization of Adsorbents and Optimization of Separation Processes
Thursday, November 2 • 11:30 AM - 12:00 PM

Use of adsorbents, both naturally occurring and synthetic, for the separation and purification of gasses has been around for many years. We will discuss the use of a commercially available dynamic breakthrough apparatus for the development and optimization of gas separation and purification processes.

Use of an Advanced Simulation Package for Predicting Breakthrough Behavior of Gas Mixtures from Single-Component Isotherms
Thursday, November 2 • 12:00 PM - 12:30 PM

We will discuss the use of a powerful dynamic simulation program, which can be used to optimize parameters and predict the competitive adsorption behavior of gas mixtures on various adsorbents.

OPEN DISCUSSION (LIGHT SNACKS WILL BE SERVED)
Thursday, November 2 • 12:30 PM - 1:30 PM

SIEMENS

Siemens PLM: Advanced Simulation to Solve & Optimize Process Development Problems
Wednesday, November 1 • 3:15 PM - 5:45 PM

A common challenge in process industries, which comprise of food, pharmaceutical, materials and biotech industries is to bring new products to market in a time and cost effective manner. Mixing is one of the most important unit operations in the production. Poor mixing can cause losses of millions of Dollars/Euros the chemical. 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.

This workshop is also open to all professors and students who would like to learn how they can use CFD in their senior projects or research projects. If you are a chemical process engineer, manager who wants to optimize current processes in ways it was never possible before, this event will help you understand the applicability of deploying simulation to achieve these objectives. If you are already using CFD in your engineering work flow, this session will demonstrate that it is not a single point simulation but rather the ability to rapidly and intelligently explore a host designs and processes that brings the most value from simulation.

NEXT GEN

Congratulations

AIChE® 35 UNDER 35

The AIChE 35 Under 35 Award was created to acknowledge the successes of AIChE young professionals, all under the age of 35, who have made significant contributions to the Institute and the chemical engineering profession and who exemplify the best of our profession in bioengineering, chemicals, education, energy, innovation, leadership and safety.


Betul Bilgin
Education


Christina Borgese
Innovation


Donna Bryant
Leadership


Elizabeth Carter
Energy


Eun Ji Chung
Bioengineering


Lane Daley
Leadership


Cole DeForest
Bioengineering


Ben Freireich
Leadership


Bala Gottimukkala
Safety


Rajamani Gounder
Education


David Holt
Leadership


Owen Jappen
Leadership


Ellen Kloppenborg
Education


Christoph Krumm
Innovation


Lucas Landherr
Education


Nastassja Lewinski
Safety


Meagan Lewis
Leadership


William Liechty
Innovation


Ali Mesbah
Chemical


Jeffery Millman
Bioengineering


Francesca Mirri
Innovation


Ruth Misener
Innovation


Holly Murphy
Bioengineering


Akash Narani
Bioengineering


Bihter Padak
Energy


Ankur Pariyani
Safety


Camille Petit
Energy


Nemoy Rau
Bioengineering

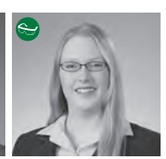

Sheena Reeves
Education


Rebekah Scheuerle
Innovation


Dawud Tan
Innovation


Ashlee Ford Versypt
Education


Matthew Webber
Bioengineering


Kendall Werts
Safety


Ahmed Youssef
Leadership

Learn more at #AIChE35Under35.

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INSTITUTE/BOARD AWARDS + MAJOR LECTURES

SUNDAY, OCTOBER 29

HONORS CEREMONY

5:30 PM — 7:00 PM • Minneapolis Convention Center, Ballroom B

Join your colleagues in honoring the recipients of the 2017 Board of Directors' and Institute Awards.

BOARD OF DIRECTORS' AWARD RECIPENTS

Founders Award for Outstanding Contributions to the Field of Chemical Engineering

Dr. William F. Banholzer
University of Wisconsin - Madison

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

(Award sponsored by The Dow Chemical Company)

Dr. Subhas K. Sikdar
U.S. Environmental Protection Agency (retired)

INSTITUTE AWARD RECIPIENTS

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

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

Dr. George W. Huber
University of Wisconsin - Madison

Alpha Chi Sigma Award for Chemical Engineering Research

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

Dr. Rakesh Agrawal
Purdue University

Andreas Acrivos Award for Professional Progress in Chemical Engineering

(Award endowed by The AIChE Foundation)

Dr. Orlin D. Velev
North Carolina State University

The Award for Service to Society

Mr. Neil Yeoman
Koch-Glitsch (retired)

3M Science. Applied to Life.™

Energy and Sustainability Award

(Award sponsored by Air Products)

3M Company
Dual Brightness Enhancement Film Team

Industrial Progress Award

Dr. Donald E. Owens III
SABIC

Industrial Research & Development Award

Dr. Robert S. Davidson
3M

Industry Leadership Award

Dr. Paul C. Collins
Eli Lilly and Company

INSTITUTE AWARD RECIPIENTS (continued)

Institute Award for Excellence in Industrial Gases Technology

(Award sponsored by Praxair, Inc.)

Dr. Phillip R. Westmoreland
North Carolina State University

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

Award inaugurated in 2017 (Award sponsored by Pfizer)

Dr. Frances Hamilton Arnold
California Institute of Technology

R. H. Wilhelm Award in Chemical Reaction Engineering

(Award sponsored by The ExxonMobil Research and Engineering Company)

Dr. Robert J. Davis
University of Virginia

Warren K. Lewis Award for Chemical Engineering Education

(Award sponsored by The ExxonMobil Research and Engineering Company)

Dr. Gintaras V. (Rex) Reklaitis
Purdue University

William H. Walker Award for Excellence in Contributions to Chemical EngineeringLiterature

(Award sponsored by John Wiley & Sons)

Dr. James B. Rawlings
University of Wisconsin - Madison

DID YOU KNOW?

The Minneapolis Institute of Art is home to one of the most impressive jade collections in the country and includes a 640-pound sculpture named Jade Mountain.

MONDAY, OCTOBER 30

MEET THE EXECUTIVES: INNOVATING FOR A SUSTAINABLE FUTURE

11:00 AM — 12:30 PM • Minneapolis Convention Center, Ballroom B ■

PANELISTS:

Sustaining Innovation/Innovating Sustainably

Dr. A.N. Sreeram
Senior Vice President & Chief Technology Officer
The Dow Chemical Company

Finding New Ways and Improved Ways Of Nourishing Our World

Dr. Chris Mallett
Corporate Vice President, Research & Development
Cargill

Creating Chemistry for a Sustainable Future

Ms. Teressa Szelest
President Market & Business Development North America
BASF

Continued Delivery on Impactful Sustainable and Innovative Business and R&D Strategies

Dr. José Méndez-Andino
Vice President, Research & Development
Owens Corning Insulation

MODERATOR:

Mr. S. Shariq Yosufzai
Vice President for Global Diversity Ombuds, University Affairs,
Chevron

■ = Supported by the AIChE Foundation

IACChE'S JAMES Y. OLDSHUE LECTURE

8:00 AM — 10:30 AM • Minneapolis Convention Center, Ballroom B

CFD Role in Understanding Mixing Processes

Dr. José Roberto Nunhez
Professor of Chemical Engineering, Head of the Computational Fluid Dynamics Laboratory
Universidade Estadual de Campinas (UNICAMP, Brazil)

DIVERSITY & INCLUSION: STARTING & THRIVING IN THE WORKPLACE

11:00 AM — 1:00 PM • Minneapolis Convention Center, 101G

PANELISTS:

Ms. Cynthia Murphy-Ortega
Manager, University Partnerships & Association Relations
Chevron

Mr. Mike McAtee
Senior Vice President Strategic Projects
BASF

Dr. Jim Sweeney
School Head Professor,
James & Shirley Kuse Chair in Chemical Engineering
Oregon State University

Ms. Yuk Louie
Manager, Process Development Division
ExxonMobil

MODERATOR:

Dr. Zenaida Gephardt
Associate Professor of Chemical Engineering
Rowan University

2017 ANDREAS ACRIVOS AWARD FOR PROFESSIONAL PROGRESS IN CHEMICAL ENGINEERING LECTURE

11:15 AM — 12:15 PM • Minneapolis Convention Center, Ballroom B ■

Engineering Amine-Modified Silicates for CO_2 Separations and Catalysis

Dr. Christopher W. Jones
Love Family Professor of Chemical & Biomolecular Engineering & Associate Vice-President for Research
Georgia Institute of Technology

■ = Supported by the AIChE Foundation

SBE'S JAMES E. BAILEY AWARD LECTURE

6:00 PM — 7:00 PM • Minneapolis Convention Center, Ballroom B

LECTURE:

Biomaterials for Tissue Engineering

Dr. Antonios G. Mikos
Louis Calder Professor of Bioengineering, Chemical & Biomolecular Engineering
Rice University

AWARD PRESENTATION:

Biotechnology Progress Award for Excellence in Biological Engineering Publication

Dr. Huimin Zhao
Steven L. Miller Chair in Chemical and Biomolecular Engineering
University of Illinois Urbana-Champaign

WEDNESDAY, NOVEMBER 1

JOHN M. PRAUSNITZ AIChE INSTITUTE LECTURE

11:15 AM — 12:15 PM • Minneapolis Convention Center, Ballroom B ■

Process Systems Engineering Contributions in Pharmaceuticals

Dr. Gintaras V. (Rex) Reklaitis
Burton and Kathryn Gedge Distinguished Professor
Purdue University

■ = Supported by the AIChE Foundation

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DID YOU KNOW?

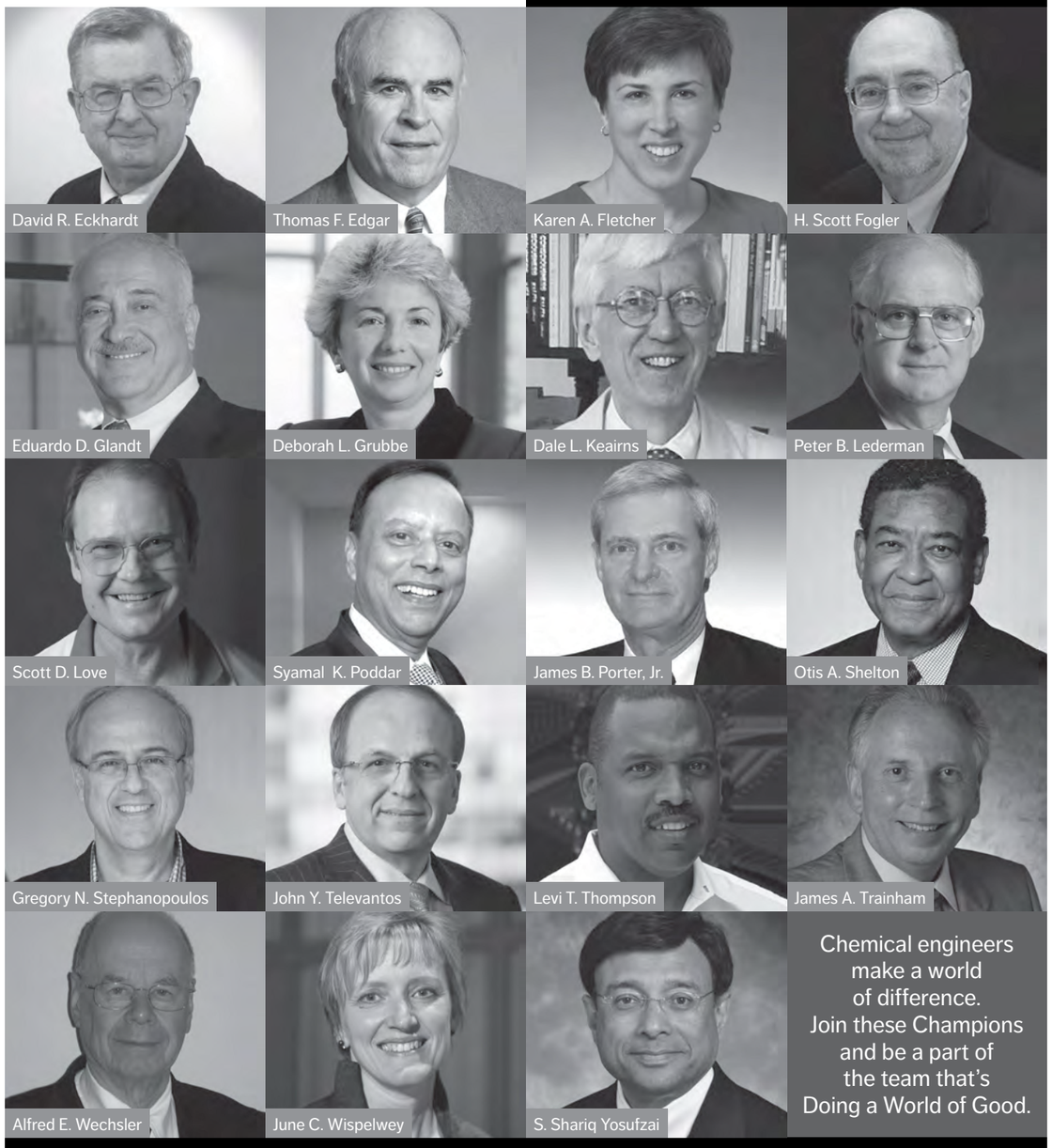
The Honeycrisp variety was invented in an apple breeding program at the University of Minnesota.

SOCIETAL IMPACT

AIChE
The Global Home of Chemical Engineers

DOING A WORLD OF GOOD

Join the Team that's Doing a World of Good



Chemical engineers make a world of difference. Join these Champions and be a part of the team that's Doing a World of Good.

To learn more and get involved visit **www.doingaworldofgood.org**.

*as of September 12, 2017

SOCIETAL IMPACT

AIChE® Foundation's Doing a World of Good Podcast

Listen in on how chemical engineers are making a positive difference to society in the latest podcast series, featuring conversations with some of the profession's most distinguished leaders.

- **Frances Arnold**, Distinguished Professor of Chemical Engineering, Bioengineering, and Biochemistry at Caltech
- **Cato Laurencin**, the Albert and Wilda Van Dusen Distinguished Endowed Chair, Professor of Orthopedic Surgery at the University of Connecticut School of Medicine
- **Gregory Yeo**, Chief Engineer at ExxonMobil Chemical Company

Visit www.aiche.org/giving/podcasts or subscribe in iTunes.

Also available in the archives:
Raj Gupta, New Mountain Capital
Edward L. Cussler, Jr., University of Minnesota
S. Shariq Yosufzai, Chevron Corporation

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AIChE® ScaleUp Program: Building Bridges between Students and Industry

AIChE Gratefully Acknowledges the 2017 ScaleUp Sponsors*

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CORNING

DOW

UOP A Honeywell Company

Objective:

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

Overview:

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

Highlights:

- Since its inception in 2007, ScaleUp has grown from 3,000 student members to over **23,000** to date.
- Since 2008, the AIChE's Safety and Chemical Engineering Education (SAChE) Certificate Program has awarded nearly **70,000** certificates to students who have demonstrated proficiency in process safety training.

To learn more about a ScaleUp corporate sponsorship, visit **www.aiche.org/giving** or contact **Ian Sergo,** Sales Director, AIChE at **ianse@aiche.org** or **646.495.1518**

*Sponsors as of August 1, 2017

Thank You to the 2017 Gold Sponsors of the AIChE® ScaleUp Program*

aspentech

www.aspentech.com

Founded in 1981, Aspen Technology is a leading supplier of software that optimizes process manufacturing in:

- Oil and gas
- Refining
- Chemicals
- Pharmaceuticals
- Engineering and construction

Our customers include over 1,500 companies spanning all process segments, as well as hundreds of universities and research labs. We have 26 offices worldwide and more than 1,200 employees working on the next generation of industry challenges.

CORNING

www.corning.com

Corning is the world leader in specialty glass and ceramics, creating and manufacturing keystone components for:

- High-technology systems for consumer electronics
- Mobile emissions control
- Telecommunications
- Life sciences

Corning succeeds as a result of sustained investment in R&D, over 150 years of materials science and process engineering knowledge, and a distinctive collaborative culture.

DOW

www.dow.com

Dow is an industry leader of specialty chemical, advanced materials, agrosciences and plastics businesses.

We believe that connecting chemistry and innovation can generate new ways to solve global challenges such as:

- Clean water
- Renewable energy generation & conservation
- Increasing agricultural productivity

We deliver technology-based products and solutions to customers in 35 countries in sectors such as electronics, water, energy, coatings and agriculture. Chemistry is changing the world and at Dow we encourage global collaboration and development.

UOP

A Honeywell Company

www.uop.com

Founded in 1914, UOP LLC products have changed the world. Today more than 60 percent of the world's gasoline and 85 percent of biodegradable detergents are made using UOP expertise.
Our refining petrochemical and gas processing technologies, products and services address shifting global demands including:

- Growing populations
- Changing environments
- Regulatory compliance challenges and more

UOP engineers have generated thousands of patents, leading to important advances within various disciplines. In addition, our latest proprietary discovery methods for identifying new catalysts and adsorbents are enabling us to bring such products to the marketplace faster than ever before.

*SPONSORS AS OF AUGUST 1, 2017

PROFESSIONAL DEVELOPMENT

CALLING ALL YOUNG PROFESSIONALS (YPs) AND GRADUATE STUDENTS:

Check out these Sessions & Events Recommended by the AIChE® Young Professionals Committee

Location: Minneapolis Convention Center

TIME	TITLE	ROOM	SPONSOR(S)
SUNDAY, OCTOBER 29			
9:00 AM - 4:00 PM	Women Grad Student and Post-doc Workshop (Ticketed)	Check the App	Women's Initiatives Committee (WIC)
9:00 AM - 4:00 PM	Women Assistant Professors and Young Scientists: Developing Your Career (Ticketed)	Check the App	Women's Initiatives Committee (WIC)
10:00 AM - 1:00 PM	AIChE Beer Brewing Competition	M100A-J	YPC
3:30 PM - 6:00 PM	Green Chemistry and Engineering	101D	Adsorption and Ion Exchange, Sustainable Energy Forum
3:30 PM - 6:00 PM	Cutting Edge and Innovative Corp and Industrial Research Proj	101H	Technology Transfer and Manufacturing, Process Research and Innovation, Research and New Technology Committee, Process Development Division
3:30 PM - 6:00 PM	Panel Speakers Forum: Chemical Process and Product Careers in Academia v. Industry	102B	Product Design, Process Intensification and Micro-process Engineering, Technology Transfer and Manufacturing, Pilot Plants, Process Research and Innovation, Process Development Division
3:30 PM - 6:00 PM	Solids Handling and Processing in the Chemical Industry: What they Don't Teach You at School	200J	Solids, Flow, Handling and Processing, Particle Technology Forum
3:30 PM - 6:00 PM	Effective Teaching for New or Prospective Faculty	205C	Education Division
5:30 PM - 6:30 PM	Graduate Student Networking Reception	Check the App	YPC
8:00 PM - 10:30 PM	Young Professionals Social ($10)	Lumber Exchange, 10 S. 5th St #300, Minneapolis, MN 55402	YPC
MONDAY, OCTOBER 30			
8:00 AM - 10:30 AM	Engineering Government Policy with a Chemical Perspective	101H	The Food-Energy-Water Nexus
9:30 AM - 10:30 AM	Networking for Nerds: How to Land (or Create) Your Dream Job and Keep Your Career Moving Forward!	101A	Publications Committee
12:30 PM - 3:00 PM	Biochemical and Biotechnical UG Research Session	101H	Nanoscale Science and Engineering Forum
12:30 PM - 3:00 PM	Solve This! Fundamental Approach to Problem Solving in Industrial Processes I	101I	Sponsored by All AIChE Divisions & Forums
12:30 PM - 3:00 PM	Undergrad Engineering Education of Ethics	L100G	Sustainable Engineering Forum, Education Division, Management Division
12:30 PM - 3:00 PM	Rapid Fire Session: TED Sep Separations Division	M100G	Separations Division
3:15 PM - 5:45 PM	Sustainability and RAPID Manufacturing Institute	101D	Sustainable Engineering Forum, Food Energy and Water Nexus, Management Division
3:15 PM - 5:45 PM	Energy and the Environment UG Research Session	101H	Sustainable Engineering Forum
3:15 PM - 5:45 PM	Solve This! Fundamental Approach to Problem Solving in Industrial Processes II	101I	Sponsored by All AIChE Divisions & Forums
3:15 PM - 5:45 PM	Use the FE Exam as an Assessment Tool?	L100G	Sustainable Engineering Forum
4:00 PM - 5:30 PM	Young Professionals Business Meeting	Check the App	YPC
TUESDAY, OCTOBER 31			
8:00 AM - 10:30 AM	Diversity and Inclusion: Starting and Thriving in the Workplace	101G	Education Division
8:00 AM - 10:30 AM	Using the Brains of Others to Innovate Faster	L100G	Management Division
8:00 AM - 10:30 AM	Tutorial Session on Electrochemical Methods, Systems and Applications	M100C	Electrochemical Fundamentals Division
12:30 PM - 3:00 PM	K-12 Outreach Activities and other Broader Impacts	101I	Education Division
12:30 PM - 3:00 PM	Finding a Healthy Work-Life Balance Amid High Stress	102C	
12:30 PM - 3:00 PM	Applied Project Management Fundamentals	L100G	Management Division
3:15 PM - 5:45 PM	Innovation From Beginning to End: Generating Ideas, Working with People, and Managing Projects	L100G	Management Division
WEDNESDAY, NOVEMBER 1			
8:00 AM - 10:30 AM	Important Issues In Professional Development Including the Management Division's Award Recipient Presentation	L100G	Environmental Division, Management Division

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For more information on each session, please use the Conference App or refer to the Meeting Program Book.

CUTTING EDGE

INTERNATIONAL CONFERENCE ON CRISPR TECHNOLOGIES

December 4-6, 2017 | Raleigh, NC

FOR BEST RATES REGISTER BY NOVEMBER 4

The International Conference on CRISPR Technologies will bring together leaders and trainees from the cutting edge of CRISPR technologies, to explore the application of those technologies to genome editing and beyond.

Session Topics Include:

- Genome editing and gene regulation in human health
- Genome editing and gene regulation in agriculture
- Genome editing and gene regulation in industrial biotechnology
- CRISPR technologies beyond genome editing and gene regulation
- Horizons of CRISPR biology
- Achieving efficient delivery and editing
- Services for CRISPR research

Featured Technical Events:

- Roundtable discussions on technical hurdles to applying CRISPR technologies in different organisms
- Panel discussion on the intersection of CRISPR technologies and society

To learn more and to register, please visit www.aiche.org/CRISPR

There are still spots open for abstracts. SUBMIT YOURS TODAY!

Conference Chairs:

- Chase Beisel, *North Carolina State University*
- Benjamin Gray, *Benson Hill Biosystems*

Organizing Committee:

- Rodolphe Barrangou, *NC State University*
- Mark Cigan, *Genus PLC*
- Gregory Davis, *Sigma Millipore*
- Kevin Esvelt, *Massachusetts Institute of Technology*
- Ryan Gill, *University of Colorado Boulder*
- Fred Gould, *NC State University*
- Sang Yup Lee, *KAIST*
- Dipali Sashital, *Iowa State University*
- Lisa Zannoni, *Syngenta*

Featured Keynote Speakers:

- Charles Gersbach, *Duke University*
- Eugene Koonin, *NIH, NCBI, NLM*

Invited Speakers:

- Omar Abudayyeh, *Broad Institute*
- Adair Borges, *University of California, San Francisco*
- Anushree Chatterjee, *University of Colorado Boulder*
- Mark Cigan, *Genus PLC*
- Jonathan Gootenberg, *Broad Institute*
- Kevin Holden, *Synthego*
- Jennifer Kuzma, *NC State University*
- Prashant Mali, *University of California, San Diego*

CRISPR TECHNOLOGIES CONFERENCE

Organized by

Society for Biological Engineering — An AIChE Technological Community

2017 TECHNICAL SESSIONS

(1) Workshop: Hands On with Molecular Simulation (Ticketed Event)
Sunday, Oct 29, 8:00 AM
MCC, 101I

Eric Jankowski, Chair
Coray M. Colina, Co-Chair

Sponsored by:
Computational Molecular Science and Engineering Forum

8:00 Paper 1a: On-Boarding Computational Scientists with Bash, Git, and Python
— Eric Jankowski

9:20 Paper 1b: MoSDeF: Molecular Simulation and Design Framework
— Christoph Klein, János Sallai, Andrew Z. Summers, Christopher R. Iacovella, Ákos Lédeczi, Clare McCabe, ***Peter T. Cummings***

10:40 Paper 1c: Managing Data Spaces, Performing MD, and Analyzing Trajectories with Signac, HOOMD-Blue, and Freud
— Carl Simon Adorf, Joshua A. Anderson, Eric S. Harper, ***Sharon C. Glotzer***

12:00 Paper 1d: How to Recognize Garbage ***— Michael Shirts***

2:00 Paper 1e: How to Use the Atomistic Monte Carlo Package Cassandra: Liquid Phase Properties and Vapor-Liquid Phase Equilibria
— Edward Maginn, *Eliseo Marin-Rimoldi, Jindal K. Shah, Ryan Gotchy Mullen*

3:20 Paper 1f: Using Python to Standardize and Format Input to Popular Molecular Simulation Software
— Coray M. Colina, *Michael E. Fortunato*

4:40 Paper 1g: Quantifying Uncertainty in Molecular Simulations
— David A. Kofke*, Andrew J. Schultz*

(2) Women Undergraduates Workshop (Ticketed Event)
Sunday, Oct 29, 9:00 AM
MCC, 101H

Heather N. Emady, Chair
Julianne L. Holloway, Co-Chair

Sponsored by:
Women's Initiatives Committee

(3) Women Assistant Professors and Young Scientists: Developing Your Career (Ticketed Event)

Sunday, Oct 29, 9:00 AM
MCC, 101G

Heather N. Emady, Chair
Julianne L. Holloway, Co-Chair

Sponsored by:
Women's Initiatives Committee

(4) Women Graduate Students and Post-Doctorates Workshop (Ticketed Event)
Sunday, Oct 29, 9:00 AM
MCC, 101F

Heather N. Emady, Chair
Julianne L. Holloway, Co-Chair

Sponsored by:
Women's Initiatives Committee

(5) Workshop: Career Planning for Prospective Faculty
Sunday, Oct 29, 10:00 AM
MCC, 101A

Tim Anderson, Chair

Sponsored by: Young Faculty Forum

(6) Chem-E-Car Competition®
Sunday, Oct 29, 12:30 PM
MCC, Exhibit Hall C

Skip E. Rochefort, Chair

Sponsored by:
Student Chapters Committee Liaison

(7) Meet the Faculty Candidate Poster Session
Sunday, Oct 29, 1:00 PM
MCC, Exhibit Hall B

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

Sponsored by: Meet the Faculty Candidate Poster Session — Sponsored by the Education Division

■ BIOMATERIALS & BIOLOGICAL ENGINEERING

Paper 7a: Organizing Biochemical Reactions with Phase-Separated Protein Droplets In Vitro and In Vivo
— Huaiying Zhang

Paper 7b: Designing Novel Surfaces to Control the Fate of Attached Microbes
— Huan Gu

Paper 7c: Drugging the Human Microbiome ***— Michael J. Fink***

Paper 7d: Kinetic of Biomass Fast Pyrolysis ***— Ali Zolghadr***

Paper 7e: Microbiome Engineering for Human Health and Agricultural Productivity ***— Collin M. Timm***

Paper 7f: Multiscale Cellular and Protein Therapeutic Engineering for the Development of Novel Immunotherapies ***— John Blazeck***

Paper 7g: Organ-on-a-Chip and 3D-Printing Technologies: Applications in Nephro-Cardiovascular Diseases
— Stella Alimperti

Paper 7h: Single-Cell Analysis Using Droplet Microfluidics ***— Leqian Liu***

Paper 7i: So This Engineer Walks into a Biology Lab: Regulating Cell Fate, Engineering Motor Neurons
— Kate E. Galloway

Paper 7j: Tissue-Engineered Models for Lymphatic and Blood Vascular Biology
— Esak Lee

Paper 7k: Understanding Bacterial Biofilms for Improved Medical and Industrial Processes ***— Erica Ricker***

Paper 7l: Biomaterial Design for Tissue Engineering, Drug/Gene Delivery and Biomedical Processes ***— Metin Uz***

Paper 7m: Creating Rechargeable Antithrombotic Surfaces for Medical Devices ***— Hyun Ok Ham***

Paper 7n: Creation of Self-Assembled Materials from Recombinant Fusion Proteins for Advanced Biomedical Platforms ***— Yeongseon Jang,*** *Julie A. Champion*

Paper 7o: Decoding the Nature-Designed Codes in Membranes: Applications in Biomedicines and Bioengineering ***— Amit Kumar Sachan***

Paper 7p: Engineering Functional Nucleic Acid Nano-Devices
— Jeffrey Vieregg

Paper 7q: Engineering Surfaces to Study Biological Interactions
— Ariel Furst*, Matthew Francis*

Paper 7r: Induction of Tolerance or Immunity by Targeting Antigens to Specific Antigen-Presenting Cells via Synthetic Polymeric Glycosylations
— Scott Wilson

Paper 7s: Materials Design via Soft-Matter Crystallography
— Julia Dshemuchadse

Paper 7t: Molecular Understanding of Physical Phenomena in Soft Materials Design and Process Development
— Qing Shao

Paper 7u: Photoautotrophic Synthesis of Designer Polysaccharides
— Cheryl Immethun

Paper 7v: Production of Artificial Cell Membranes Bearing New Characteristics or Behaviors Using "Click" Chemistries
— Danielle Konetski*, Dawei Zhang, Austin Baranek, Tao Gong, Brady Worrell, Christopher Bowman*

Paper 7w: Self-Organization in Soft, Active Materials
— Kimberly L. Weirich

Paper 7x: Tough-Gradient Double-Network Hydrogels for Artificial Implants
— Pandiyarajan Chinnayan Kannan

Paper 7y: Transcriptome-Guided Cell and Gene Therapy Strategies to Treat Neurodegeneration
— Maroof M. Adil

Paper 7z: Cancer Immunotherapy, Cell Imaging and Drug Delivery from Self-Assembled Structure
— Jae-Ho Lee

Paper 7aa: Engineering Optical Nanomaterials for Biological Sensing and Imaging
— Jackson Travis Del Bonis-O'Donnell

Paper 7ab: Biopolymers Produced by a Thermophile *Geobacillus* sp. WSUCF1
— Jia Wang*, David R. Salem, Rajesh K. Sani*

Paper 7ac: Cell-Free Biotechnology for a Low-Carbon Future
— Joseph Rollin

Paper 7ad: Harnessing Diverse Microorganisms for Biochemical Production Using Carbon Dioxide
— Jason T. Boock

Paper 7ae: Streamlining Chemical Process Design with Process Systems Engineering Methods
— Kefeng Huang

Paper 7af: Nano-Bio-Sensors for Point-of-Care Diagnostics
— Sahar S. Mahshid

Paper 7ag: Novel Biosensors for Transformative Healthcare
— Yunshan Wang

Paper 7ah: Polymer-Based Nano-Sensing Technology Platforms for Healthcare, Environmental Monitoring
— Ramchander Chepyala

Paper 7ai: Uncovering Cellular Heterogeneity in Complex Tissues Through Single-Cell Transcriptomics: Structure, Development, and Dysfunction — ***Karthik Shekhar***

Paper 7aj: Engineering Ligands to Control Protein Conformational Changes — ***Daniel R. Woldring***

Paper 7ak: Engineering Next-Gen Proteases as Therapeutics and as Tools in Biomedicine and Synthetic Biology — ***Carl A. Denard***, *Brent L. Iverson*

Paper 7al: Exploiting Organization in Bacteria for Synthetic Biology — ***Edward Y. Kim***

Paper 7am: Leveraging Big Data and Engineering Fundamentals Towards Rational Biological Discovery — ***Purushottam Dixit***

■ BIOMEDICAL ENGINEERING

Paper 7an: Micro-Scale Transport Processes Enable Accelerated Biochemistry, Chaotic Mixing and Inexpensive Mobile Diagnostics — ***Aashish Priye***

Paper 7ao: Complex Fluids in Complex Small-Scale Geometries — ***Hamed Haddadi***

Paper 7ap: Design and Development of Ocular Disease Diagnostic System, and Point-of-Care Microsystem — ***Jae Hwan Jung***

Paper 7aq: Electrokinetic Analytical Tools for Cell Characterization and Biosensing Technology — ***Tayloria N. G. Adams***

Paper 7ar: Engineering Devices for Diagnostics, Therapeutics and Discovery Science — ***Suman Bose***, *Robert Langer, Daniel G. Anderson*

Paper 7as: Engineering Vascularized Organ-on-Chip Systems to Advance Biological Understanding and Therapeutic Intervention in Human Cancer and Blood Stem Cell Biology — ***Duc-Huy Nguyen***

Paper 7at: Genetic Engineering of Immune Cell Recruitment to Control Inflammation — ***Alexander Buffone Jr.***

Paper 7au: Imran Rizvi, Ph.D. Assistant Professor, Department of Dermatology, Harvard Medical School; And Assistant Biomedical Engineer, Wellman Center for Photomedicine, Department of Dermatology, Massachusetts General Hospital — ***Imran Rizvi***

Paper 7av: Micro-/Nano-Fabrication and 3D-Bioprinting Technologies: An Engineering Approach Toward Translational Medicine — ***Pooya Davoodi***, *Chi-Hwa Wang*

Paper 7aw: Molecular-Level Analysis of the Serological Antibody Repertoire — ***Jiwon Lee***

Paper 7ax: Stochasticity, Complexity, and Multiscale Dynamics in Cancer Progression and Drug Response — ***Leonard A. Harris***

Paper 7ay: Multiscale Multiphysics Modeling of Blood Clotting and Thrombus Biochemomechanics in the Vasculature — ***Alireza Yazdani***

Paper 7az: Synthetic Polypeptide-Assisted Assembly of Ribonucleoproteins for Enhanced Delivery of SiRNAs and mRNAs — ***Jiahe Li***, *Wade Wang, Connie Wu, Yanpu He, Yingzhong Li, Darrell J. Irvine, Paula Hammond*

Paper 7ix: Utilization of Lignocellulosic Biomass to Value-added Bio-products — ***Chang Geun Yoo***

Paper 7iy: Leveraging Physiological Microenvironment to Transport across Biological Barriers — ***Sufeng Zhang***

Paper 7ja: Methods for Efficient Sequence to Activity Mapping — ***Gur Pines***

■ METABOLIC ENGINEERING

Paper 7ba: Enabling C1-Based Bioconversion Through Metabolic Engineering — ***Benjamin Woolston***

Paper 7bb: Engineering Metabolism for Carbon Conservation and Cellulosic Biofuel Production— ***Paul Lin***

Paper 7bc: From Integrative Metabolomics to Understanding Human Diseases and Enhancing CO_2 Fixation — ***Junyoung O. Park***

Paper 7bd: Genetically Portable Synthetic RNA Biology Tools for Metabolic Engineering — ***Richard A. Lease***

Paper 7be: Selective Expansion of the Microbial Chemistry Repertoire for Metabolic and Protein Engineering — ***Aditya M. Kunjapur***, *Kristala L. J. Prather, George M. Church*

■ SYNTHETIC BIOLOGY

Paper 7bf: Application of Synthetic Biology Toward Environmental and Biomedical Applications — ***Qing Sun***

Paper 7bg: Design of Synthetic C1 Carbon Assimilation Pathways — ***Hong Yu***

Paper 7bh: Genome- and Biome-Scale Microbial Engineering Using Synthetic Biology, Robotic Automation, and Mass Spectrometry Imaging — ***Tong Si***

Paper 7bi: Synthetic Biology for Next-Generation Plant Natural Product Discovery and Biosynthesis — ***Sijin Li***, *Christina D. Smolke*

■ PHARMACEUTICALS

Paper 7bj: Developing Biologically Active Ionic Liquids for Therapeutic Applications — ***Wilmarie Medina-Ramos***

Paper 7bk: Pharmaceutical System Engineering — ***Ravendra Singh***

■ PARTICLE TECHNOLOGY

Paper 7bl: Programmable Soft Matter for Active Reconfiguration, Biotransport and Delivery — ***C. Wyatt Shields IV***

Paper 7bm: Synthesis of Core-Shell Microparticles Containing Thermoset Resins via Suspension Polymerization — ***Guozhen Yang***, *Mengfei Huang, John Klier, Jessica D. Schiffman*

Paper 7bn: The Mesoscopic Physics of Discrete Media: Towards the Control of Dynamic Structures — ***Victor Francia***

■ POLYMERS

Paper 7bo: Engineering Precision Polymers for Advanced Applications — ***Jimmy Lawrence***

Paper 7bp: Advanced Biologic-Synthetic Composites — ***Rachel A. Letteri***

Paper 7bq: Building New Materials and Electronics Within Intact, Living Biological Systems: From Nanoelectronics Through Polymeric Devices to Genetically Targeted Electronics — ***Jia Liu***

Paper 7br: Deep Learning in Chemical Engineering — ***Amir Barati Farimani***

Paper 7bs: Exploiting Interfacial Phenomena and Non-Equilibrium Assembly in Polymeric Materials — ***Katherine P. Barteau***

Paper 7bt: From Soft Materials to Soft Circuits — ***Xiaoxue Wang***

Paper 7bu: Intrinsically Stretchable Skin Electronics for Wearable Biomedical Applications — ***Sihong Wang***

Paper 7bv: Molecular Simulations of Gas Transport in Polymer Membranes — ***Kai Zhang***, *Sanat Kumar*

Paper 7bw: Electrically Conductive Nanomaterials and Their Multifunctional Polymeric Nanocomposites for Energy, Health, and Environment — ***Mohammad Arjmand***, *Uttandaraman Sundararaj*

Paper 7bx: Nanorheology of Entangled Polymer Melts — ***Ting Ge***, *Gary S. Grest, Michael Rubinstein*

Paper 7by: Polymer Process Design and Modelling to Fabricate and Understand Unique Composite Architectures — ***Alex M. Jordan***

Paper 7bz: Polymer/Graphene Oxide Thermosets with Multifunctional GO as a Crosslinker— ***Heonjoo Ha***

Paper 7ca: Programmable Assembly and Deformation of Polymers and Networks— ***Jinhye Bae***

Paper 7cb: Structure–Property Relationships in Polymer-Based Transistors — ***Seung Hyun Sung***

Paper 7cc: Three-Dimensional Responsive Soft Micro/Nano-Structures for Biomedical and Electronic Applications — ***Weinan Xu***, *David H. Gracias*

■ MATERIALS

Paper 7cd: Functional Materials Interfacing Chemistry and Biology — ***Weixia Zhang***

Paper 7ce: Plasmonic Perovskites Nanolasers in Accelerating Emission Dynamics— ***Sui Yang***

Paper 7cf: First-Principles Study for Detailed Understanding of Nanoporous Materials — ***Joshua D. Howe***

Paper 7cg: Colloidal Assemblies for Mesoscale Materials — ***Katherine Phillips***

Paper 7ch: Colloidal Fluids as Electrical Current Collectors — ***Jeffrey J. Richards***

Paper 7ci: Complex Fluids and Anisotropic Liquids for Molecular Engineering and Rational Material Design — ***Monirosadat Sadati***

Paper 7cj: Contorted Molecular Semiconductors for Organic Electronics — ***Yu Zhong***, *Michael Steigerwald, Xiaoyang Zhu, Fay Ng, Colin Nuckolls*

Paper 7ck: Controlling the Dynamics of Soft Materials at Interfaces — ***Siddarth Srinivasan***

Paper 7cl: Design of Advanced Materials by Using Ab-Initio Structural Search — ***Irais Valencia-Jaime***

Paper 7cm: Endowing Metal-Organic Framework (MOF) Materials with Scale-Up Production, Functionality, and Processability for Gas Separation and Heterogeneous Catalysis — ***Zhigang Hu***

Paper 7cn: Engineered Porous Materials for Advanced Chemical Conversions: Understanding Structure-Property-Acitivty Relationship — ***Satish K. Nune***

Paper 7co: Engineering Materials and Devices for Energy, Environment and Human Health: From Capillary Foams to Wearable Sensors and Implantable Neural Probes — ***Yi Zhang***

Paper 7cp: Engineering Molecular Interactions in Biological and Electrochemical Interfaces — ***Matthew A. Gebbie***

Paper 7cq: Engineering Precision Polymers for Advanced Materials Applications — ***Amanda B. Marciel***

Paper 7cr: Fabrication of Functional Nanofibers and Hydrogels: Gelation Behavior and Viscoelasticity of Polymer Solutions — ***Tomoki Maeda***

Paper 7cs: Metallurgy-Mimic Thermal Processing and Morphology of Particle-Forming Diblock Copolymers — ***Kyungtae Kim***, *Frank S. Bates*

Paper 7ct: Nuclear Spin Hyperpolarization for Characterization of Materials, Surfaces, and Interfaces — ***Jonathan King***

Paper 7cu: Porous Materials Chemistry for Catalysis and Separations — ***Simon H. Pang***

Paper 7cv: Self-Aligned Strategies for Printed Electronics — ***Woo Jin Hyun***

Paper 7cw: Skin Layer Formation During Drying of Latex Films — ***Hao Huang***

Paper 7cx: Socially Responsible Hybrid Materials: From Molecular Engineering to Practical Applications — ***Nader Taheri Qazvini***

Paper 7cy: Synthesis of Crumpled Graphene-Based Materials Using Aerosol Techniques and Their Application to CO_2 Photoreduction — ***Yao Nie***

Paper 7cz: Targeted Design of Next-Generation Materials — ***Hadi Ramezani-Dakhel***

Paper 7da: The Crystal Quality and Structure of AM-6 — ***Rumeysa Tekin***, *Juliusz Warzywoda, Albert Sacco Jr.*

Paper 7db: Theoretical and Computational Study of Soft Matter Systems: From Classical Challenges to Rational Design of New Materials — ***Rui Wang***

Paper 7dc: Vapor-Phase Deposition for Functional Metal-Organic Framework (MOF) and Polymer Thin Films — ***Junjie Zhao***

Paper 7dd: Computational Design of Surfaces and Nanostructures for Energy Applications — ***Matthew M. Montemore***

Paper 7jc: Experimental Interrogation of Polymer Material Structure-Property Relationships — ***Richard J. Sheridan***

■ NANOMATERIALS & NANOTECHNOLOGY

Paper 7de: A Marriage of Convenience: Uniting Polymer Chemistry and Polymer Physics to Craft Advanced, Functional Materials — ***Robert C. Ferrier Jr.***

Paper 7df: Beyond Graphene: Two-Dimensional Transition Metal Carbides and Nitrides (MXenes) — ***Meng-Qiang Zhao***, *Chang Ren, Babak Anasori, Yury Gogotsi*

Paper 7dg: Biomolecular Sensing Using Fluorescent Single-Wall Carbon Nanotubes — ***Juyao Dong***

Paper 7dh: Interaction of Nanostructures Leads to Macroscopic Behaviors: Towards Designing Multiple-Component Nanostructures with Functionalities for Energy-Related Applications — ***Fen Qiu***

Paper 7di: Light and Heat-Managing Nanomaterial for Energy Efficiency and Human Health — ***Po-Chun Hsu***

Paper 7dj: Multiscale Design of Heterogeneous Nanomaterials for Energy Applications: Solution Synthesis, Structures, and Properties — ***Haoran Yang***

Paper 7dk: Rational Materials Design for Energy and Heterogeneous Catalysis Applications: Noble Metal Single-Atom Catalysts and 1D Nano-Array Support Materials — ***Son Hoang***

Paper 7dl: Smart Magnetic Nanomaterials for Sustainable Applications in Biomedicine and Catalysis — ***Ayomi S. Perera***

Paper 7dm: Solution-Processable Multicomponent Nanomaterial for Next-Generation Transparent Electronic/Optoelectronic Devices — ***Ajay Singh***

Paper 7dn: Tunable Hygromorphism: Structural Implications of Molecular Gels and Electrospun Nanofibers in Bilayer Composites — ***Symone Alexander***

Paper 7do: Ubiquitous Energy Harvesting Through Chemically Engineered 2D Materials — ***Xu Zhang***

Paper 7dp: Understanding and Controlling Interfaces of Nanomaterials via Electrochemistry — ***Tuncay Ozel***, *Chad A. Mirkin, Daniel G. Nocera*

Paper 7dq: Directed Self-Assembly of Blue Phases Single Crystal by Chemically Patterned Surfaces — ***Xiao Li***, *Jose Martinez-Gonzalez, Ye Zhou, Monirosadat Sadati, Rui Zhang, Juan de Pablo, Paul F. Nealey*

Paper 7dr: Multifunctional Soft-Nano Interfaces for Energy, Environment, and Healthcare — ***Kunal Mondal***, *Michael D. Dickey, Ashutosh Sharma, Jan Genzer*

Paper 7ds: Advanced Materials and Nanotechnologies for Water-Energy Applications — ***Chong Liu***

Paper 7dt: Liquid-Phase Characterization, Modification, and Controlled Assembly of Novel 2D Nanomaterials — ***Dorsa Parviz***

Paper 7du: Multiscale Design of Aerosol Synthesis of Nanomaterials — ***Eirini Goudeli***

Paper 7dv: Nano-Material-Based Protein Sensor Design for Complex Cellular Environments by a Fast-Integrated Simulation System — ***Shuai Wei***

Paper 7dw: Optimizing Polymeric Nanoparticle Synthesis for Drug Delivery Using Experimental Design — ***Amber C. Jerke***

Paper 7dx: Patterning and Actuating Soft Materials Towards Functional Surfaces and Devices — ***Sungjune Park***

Paper 7dy: Sustainability Through Nanoscience: Green, Smart, and Controllable Synthesis and Characterization of One-Dimensional Metal Nanostructures — ***Shohreh Hemmati***

Paper 7dz: Wearable/Implantable Ultrathin Electronic/Optoelectronic Devices with Engineered Semiconductor Nanocrystals — ***Hyeong Jin Yun***

■ CATALYSIS

Paper 7ea: Monolithic Catalyst for Sustainable Ammonia Synthesis at Low Temperature — ***Giovanny Mateus***, *Andrea Ariman*

Paper 7eb: A Holistic Design Approach for Zeolite Catalysts — ***Florian Göltl***

Paper 7ec: Catalysis for Energy: Catalyst Design Based on Spectroscopy and Fundamental Structure-Function Relationships — ***Konstantinos A. Goulas***

Paper 7ed: Catalytic Biomass Conversion — ***Jiaguang Zhang***

Paper 7ee: Computational-Driven Strategies for the Rational Design of Novel Catalysts for Clean Energy Generation and Fuel Synthesis — ***Shyam Kattel***, *Ping Liu, Jingguang G. Chen*

Paper 7ef: Data-Driven Catalyst Design and Optimization — ***Yongchun Hong***

Paper 7eg: Designing Multicomponent Nanostructured Materials for Energy Storage and Conversion — ***Gregory S. Hutchings***

Paper 7eh: Developing Fundamental Insights into Heterogeneous Catalytic Reactions for Selective Chemical Production and Sustainable Fuels — ***Matthew Kale***

Paper 7ei: Efficient Catalytic Pathways for Carbon Utilization and Emission Control Technologies — ***Erdem Sasmaz***

Paper 7ej: Enabling New Reaction Pathways Through Creation of Tailored Molecular Sieve Catalysts — ***Viktor J. Cybulskis***

Paper 7ek: Enhanced Catalytic Capability Through Controlled Reaction Environments: A Merger of Solvent Effects and Rational Catalyst Design — ***Omar A. Abdelrahman***

TECHNICAL SESSIONS 2017

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Paper 7el: Enhanced Stability for Propene Epoxidation with H_2 and O_2 on Au Catalysts Supported on Nanosheets TS-1 — ***Nan Sheng***

Paper 7em: Explaining Surface-Catalyzed Reactions in Electrochemistry — ***Eric Walker***

Paper 7en: Insight and Applications of Pt-Bi Bimetallic Catalysts: A Combined Experimental and DFT Study — ***Yang Xiao***, *Arvind Varma*

Paper 7eo: Integrating Computational Chemistry Techniques to Understand Complex Chemical Reactions — ***Tibor Szilvási***

Paper 7ep: Integration of Machine-Learning and Data-Management Methods for Accelerated Catalyst Modeling and Exploration — ***Jacob R. Boes***

Paper 7eq: Magnetic Polymer Nanocomposites for Giant Magnetoresistance and Electromagnetic Shielding — ***Jiang Guo***, *Alexandra Galaska, Brian J. Edwards, Bamin Khomami, Zhanhu Guo*

Paper 7er: Making Renewables Chemicals and Biofuels Economical: Toward Complete Utilization of Lignocellulosic Biomass — ***David Martin Alonso***

Paper 7es: Mechanisms of Heterogeneous Catalysis for Clean Energy Conversion and Efficient Chemical Production — ***Luke Neal***

Paper 7et: Modification of Nickel-Based Catalysts for the Dry Reforming of Methane by Atomic Layer Deposition — ***Patrick Littlewood***, *Mike Liu, Eric Weitz, Neil M. Schwietzer, Tobin J. Marks, Peter C. Stair*

Paper 7eu: Molecular Modelling for Catalytic Reaction Engineering — ***Jithin John Varghese***

Paper 7ev: Nanoscale Engineering of Electrocatalysts Using Atomistic Modeling — ***Joseph H. Montoya***

Paper 7ew: Novel Approaches for Carbon-Neutral Energy Conversion — ***Zhi Cao***

Paper 7ex: Rational Design of Material Interfaces for Electrochemical Energy Conversion and Storage — ***Ming Gong***

Paper 7ey: Renewable Bulk Chemicals Production Using Porous Catalytic Materials: A Mechanistic Perspective — ***Sha Li***

Paper 7ez: Solar Energy Conversion via Photovoltaics and Photocatalysis — ***Won Jun Jo***, *Jae Sung Lee, Karen Gleason*

Paper 7fa: Structure-Function Relations in Bifunctional Catalysis: Kinetic, Spectroscopic, and Theoretical Approaches — ***Gina Noh***

Paper 7fb: Supported Molybdenum Dio-Oxo Catalysts for Acceptorless Aqueous Alcohol Dehydrogenation — ***Tracy Lohr***, *Neil M. Schwietzer, Peter C. Stair, Tobin J. Marks*

Paper 7fc: Surface Interactions of High-Performance Materials for Energy-Efficient Technologies — ***Zenda D. Davis***

Paper 7fd: Synthesis of Organometallic Single-Site Heterogeneous Catalysts for Sustainable Chemistry — ***Jacob Heltzel***, *Adelina Voutchkova-Kostal*

Paper 7ff: Understanding and Improving Heterogeneous Catalysis for Sustainable Production of Renewable Fuels and Chemicals — ***Jiayue He***

Paper 7fg: Methane Oxidation over, and Regeneration of, Sulfur-Treated Bimetallic Pd/Pt Catalysts — ***Monique Shauntá Wilburn***, *William Epling*

Paper 7fh: Structure-Function Correlations of Nanomaterials in Heterogeneous Catalysis — ***Weiqing Zheng***

Paper 7fi: Advanced Functional Porous Materials as Heterogeneous Catalysts — ***Masoudeh Ahmadi***

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Paper 7fj: Designing Solid-Liquid Interphases and Polymer Composite Networks for Energy Storage and Carbon Capture — ***Snehashis Choudhury***

Paper 7fk: Electrodeposition-Based Additive Manufacturing: Combining Bipolar Electrochemistry with Scanning Probe Methodology for Freeform Fabrication — ***Trevor M. Braun***

Paper 7fl: Engineering the Next Generation of Electrochemical Energy Storage — ***Kevin Knehr***

Paper 7fm: Stable Electrochemical Growth in Viscoelastic Electrolyte — ***Shuya Wei***, *Lynden A. Archer*

Paper 7fn: Designing Electrochemical Surfaces and Interfaces for Catalysis, Separation Membranes, and Sensors — ***Jesse D. Benck***

■ SEPARATIONS

Paper 7fo: Adsorption of Copper and Nickel from Wastewater in Fixed Bed Using Bentonite Clay — ***Saad Aljlil***

Paper 7fp: Investigating Kinetics Under Extremely Harsh Conditions for Energy and Food Processing — ***Xiao-Yu Wu***

Paper 7fq: Molecule Separation and Conversion Using Novel Porous Material — ***Jian Liu***

Paper 7fr: Applying CVD Polymers in Membrane Separation, Biomedical Devices and Soft Electronics — ***Minghui Wang***

Paper 7fs: Mechanistic, Spectroscopic and Theoretical Assessment of Porous Catalytic Materials — ***Michele L. Sarazen***

Paper 7ft: Membrane Separations for Clean Energy Conversions — *Simona Liguori*

Paper 7fu: Membranes as Phase Contactors and Catalytic Interfaces — ***John P. Stanford***

Paper 7fv: Nanoporous Ultrathin-Skinned Hollow Fiber Membranes — ***Chen Zhang***

Paper 7fw: Microporous Inorganic and Composite Membranes for Energy-Efficient Separations — ***Xiaoli Ma***

Paper 7fx: Molecular Design of Redox-Active Electrochemical Interfaces: Selective Separations and Beyond — ***Xiao Su***

Paper 7fy: Bio-Mimetic Membranes for Energy-Efficient Clean Water Processes — ***Steven T. Weinman***

■ ENERGY & SUSTAINABILITY

Paper 7fz: Renewable Transportation Biofuel and Value-Added Chemical Production from Wet Biowaste — ***Wan-Ting Chen***

Paper 7ga: Metal Oxide Redox Materials for Energy Applications — ***Peter Kreider***

Paper 7gb: A Review of Recent Advances in Cost-Effective Infrastructure System Design of the CO_2 Distribution to Multiple CCS Injection Wells — ***Hossein Dashti***, *Jim Underschultz, Andrew Garnett, Victor Rudolph*

Paper 7gc: Atomistic Modeling of Energy Storage Materials — ***Jeffrey S. Lowe***, *Donald J. Siegel*

Paper 7gd: Convergence as a Chemical Engineering Career — ***Cory Jensen***

Paper 7ge: Developing Energy Materials Through New Material Synthesis and Advanced Optoelectronic Characterization — *Charles J. Hages*

Paper 7gf: From Fundamental Understanding Towards Materials Design of High-Energy Battery Materials — ***Yuzhang Li***, *Yi Cui*

Paper 7gg: Investigation and Implementation of Adsorption Models in Nuclear Energy — ***Austin Ladshaw***, *Sotira Yiacoumi, Costas Tsouris*

Paper 7gh: Mechanical Principles of Biofilm Formation — ***Jing Yan***, *Bonnie Bassler, Ned Wingreen, Howard A. Stone*

Paper 7gi: Multi-Level Systems Modeling — ***Emre Gençer***

Paper 7gj: Ion Transport in Charged Porous Media: From Porous Electrodes to Geological Flows — ***Mohammad Mirzadeh,*** *Frederic Gibou, Todd M. Squires, Martin Z. Bazant*

Paper 7gk: Modeling of Light-Driven Heterogeneous Catalysis and Other Excited-State Processes at the Nanoscale — ***John Mark P. Martirez***

Paper 7gl: Transitional Solutions Towards Decarbonized Economy — ***Mohammad S. Masnadi***

Paper 7gm: Pore-Level Multiscale Simulation of SAGD — ***Peyman Mohammadmoradi***, *Apostolos Kantzas*

Paper 7gn: Nanoscale Fluid Transport in Subsurface Energy and Water-Energy Nexus Applications — ***Tuan Ho***

Paper 7go: Screening Improved Recovery Methods in Tight Oil Formations by Injecting and Producing Through Fractures — ***Harpreet Singh***

Paper 7gp: Aerosol Synthesis of Materials for Sunlight-Harvesting Applications — ***Shalinee Kavadiya***

Paper 7gq: Harvesting, Conversion, and Direct Utilization of Solar Energy — ***Umar Aslam***

Paper 7gr: Solution-Processed Optoelectronics: Materials to Devices — ***Jeffrey A. Christians***

Paper 7gs: Integrated Modeling for Solutions in Carbon Management — ***Peter C. Psarras***

Paper 7gt: Influence of Radioactivity-Induced Charging on Global Transport of Radioactive Aerosols Released During the Fukushima Daiichi Nuclear Power Plant Accident — ***Yong-ha Kim***, *Sotira Yiacoumi, Athanasios Nenes, Costas Tsouris*

■ PROCESS DESIGN, DEVELOPMENT, & CONTROL

Paper 7gv: Advanced Control for Next-Generation Materials Synthesis and Smart Manufacturing — ***Joel Paulson***

Paper 7gw: Data-Driven Modeling and Control for Engineering Next-Generation Processes — ***Robert J. Lovelett***

Paper 7gx: Discrete and Hybrid Dynamics, Cyber-Physical Systems, and Formal Methods in Chemical Engineering — ***Blake C. Rawlings***

Paper 7gy: Novel Strategies for Quantification of Model Uncertainty and Real-Time Optimization of Batch Operations — ***Francesco Rossi***, *Gintaras Reklaitis, Flavio Manenti, Guido Buzzi-Ferraris*

Paper 7gz: Development and Assessment of New Processes for the Production of Bio-Products — ***Sampath Gunukula***

Paper 7ha: Investigating Continuous Biochemical Processing Strategies Utilizing Process Systems Engineering Fundamentals — ***Jonathan P. Raftery***

Paper 7hb: Process Systems Engineering in Pharmaceutical Process Development — ***Qinglin Su***

Paper 7hc: Process Systems Engineering Methods in the Design and Optimization of Biorefineries and the Supply Chain — ***Athanassios Nikolakopoulos***

Paper 7hd: Scientific Computing and Mathematical Modelling for Multiscale Nonlinear Systems — ***Amir Akbari***

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Paper 7hg: Solvation Behavior of Self-Assembled Systems: Investigating the Colloidal Interface via Molecular Simulations — ***Kevin R. Hinkle***

■ FLUID MECHANICS

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Paper 7hi: Chemistry and Physics of Biological Fluids on the Mesoscopic Scale — ***Jesper J. Madsen***

Paper 7hj: Interfacial Transport Phenomena with Applications to the Environment and Human Health — ***Jie Feng***, *Howard A. Stone, Robert K. Prud'homme*

Paper 7hk: Microscale Flows: With Applications in Nanofluidics, Active Matter, and Rheology — ***Sarit Dutta***

Paper 7hl: Modeling Liquid Crystals, Active Matter and Other Non-Equilibrium and Nonlinear Soft Materials — ***Rui Zhang***

Paper 7hm: Multiphase Interactions to Create Designer Material — ***Sara Moghtadernejad***

Paper 7hn: Spherically Confined Colloidal Suspensions of Hydrodynamically Interacting Particles: A Model for Intracellular Transport — ***Christian Aponte-Rivera***

Paper 7iz: Reduced-order Transport Models for Energy and the Environment — ***Zhong Zheng***

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Paper 7hp: Controlling and Characterizing Complex Fluid-Fluid Interfaces — ***Javen Weston***

Paper 7hq: Engineering Metal Surfaces via Electrochemical Reactions for Advanced Functionalities — ***Won Tae Choi***

Paper 7hr: Explore Colloidal and Interfacial Phenomena in Complex Fluids: From Isolated Fluid Particles to Their Close Packing Structures — ***Nan Shi***

Paper 7hs: Tailoring Functionality from Disorder: Complex Nonequilibrium Phenomena at Biological and Nanomaterial Interfaces — ***Alexander J. Pak***

Paper 7ht: Computational Micro/Nanofluidics — ***Xikai Jiang***, *Rui Qiao, Olle G. Heinonen, Juan J. de Pablo*

Paper 7hu: Imaging the Structure and Dynamics of Soft Materials — ***Yi Peng***

Paper 7hv: In-Silico Design of Ionic Liquid Adducts for Biomedical and Electrochemical Applications — ***Fardin Khabaz***

Paper 7hw: Modeling Across Disparate Spatiotemporal Scales – Enabling Answers to Grand Engineering Challenges — ***Dwaipayan Dasgupta***

Paper 7hx: Spin-Segregation of Active Spinners — ***Somayeh Farhadi,*** *Paulo E. Arratia, Douglas J. Durian*

Paper 7hy: Application of Ultrasound for Synthesis of Carbon Capture Microcapsules — ***Srinivas Mettu***

Paper 7hz: Curvature Matters: Reconfigurable Materials from Anisotropic Colloid Interactions — ***Isaac Torres-Diaz***

Paper 7jb: Colloidal and Interfacial Phenomena Involving Anisotropic Fluid — ***Xiaoguang Wang***

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Paper 7ib: Computational Modeling of Catalytic Reactions and Nanomaterials: Mechanisms and Structure-Function Relationships — ***Wei Lin***

Paper 7ic: Correlating Structure and Performance of Heterostructured Materials for Energy Generation and Storage — ***Liang Zhang***

Paper 7id: Materials and Methods for Sustainable CO_2 Conversion Towards Hydrocarbon Generation — ***Debtanu Maiti***

Paper 7ie: Molecular Modeling and Machine Learning for Catalysis and Separations — ***Tyler R. Josephson***

Paper 7if: Molecular Modeling of Anti-Microbial Peptides at Water-Membrane Interface — ***Faramarz Joodaki***

Paper 7ig: Multiscale Modeling of Liquid Solutions and Solid-Liquid Interfaces — ***Nav Nidhi Rajput***

Paper 7ih: Multiscale Simulations of Nonequilibrium Mechanisms in Aqueous Solutions — ***Aviel Chaimovich***

Paper 7ii: Predictive Bottom-Up Design of Nanomaterials for Biomimicking Applications — ***Trung Nguyen***

Paper 7ij: Wave Function–Based Framework for Computational Catalyst Discovery — ***Alexander V. Mironenko***

Paper 7ik: Data Analytics for Complex Systems — ***Kristen Severson***

Paper 7il: Dynamic Systems Spanning Engineering to Medicine — ***Anwesha Chaudhury***

Paper 7im: Global Optimization Techniques for System Identification and Green Engineering Applications — ***Jeremy A. Conner***

Paper 7in: Multi-Physics Modeling and Parallel Computing in Biological Flows — ***Jifu Tan***

Paper 7io: Multiscale Optimization in Process Systems Engineering — ***John P. Eason***

Paper 7ip: Multiscale Processes Intensification and Optimization of Process Systems — ***Flavio da Cruz***

Paper 7iq: Optimization-Based Control of Complex Process Networks: Application to Medicine and Energy Systems — ***Davood Babaei Pourkargar***

Paper 7ir: Process Systems Engineering for Transforming Industrial Flares into a Source of Energy by Managing Uncertain Abnormal Situation — ***Monzure-Khoda Kazi***

Paper 7is: Modeling Chemical Reactivity for Nanoscale Design — ***Ryan Gotchy Mullen***

Paper 7it: Computational Design and Characterization of Nanoscale Materials for Energy Applications — ***N. Scott Bobbitt***

Paper 7jd: Level Seet Algorithms for Polymer Field Theory — ***Gaddiel Ouaknin***

■ EDUCATION

Paper 7iu: High-Performance Computing Approaches to Large-Scale Stochastic Programming and Data Analysis — ***Yankai Cao***

Paper 7iv: Water/Solute Permselectivity Limits of Biomimetic Desalination Membranes — ***Jay Werber***, *Menachem Elimelech*

Paper 7iw: Conducting Flow-Induced Crystallization Studies on Flexible and Semi-Rigid Polymers: A Facilitator of Education in Polymer Physics
— ***Behzad Nazari***

(8) Public Affairs and AIChE: A PAIC Town Hall
Sunday, Oct 29, 3:30 PM
MCC, 102A

Phillip R. Westmoreland, Chair

Sponsored by:
Public Affairs and Information Committee

3:30 Paper 8a:
Introductory Remarks by Nada Anid
— ***Nada Marie Anid***

3:45 Paper 8b:
Food-Energy-Water Issues
— ***Dale Keairns***

4:00 Paper 8c:
Advanced Manufacturing
— ***Raymond Adomaitis***, *Ka Ng*

4:15 Paper 8d:
Climate Change Review and Adaptation
— ***Mary Ellen Ternes***

4:30 Paper 8e: PAIC Town Hall
— ***Nada Marie Anid***

(9) Accelerated Discovery and Development of Inorganic Materials
Sunday, Oct 29, 3:30 PM
MCC, 209A/B

Sankar Nair, Chair
Yongchul G. Chung, Co-Chair
Dongxia Liu, Co-Chair

Sponsored by: Inorganic Materials

3:30 Paper 9a: New Milestones and Challenges in High-Throughput Computation of Elastic Properties on the Materials Project
— ***Joseph H. Montoya***, *Kristin Persson*

3:51 Paper 9b: Breaking Badly: A Comprehensive Assessment of Computational Methods for Predicting Tensile Strengths in Bulk Solids
— ***Bryan M. Wong***

4:12 Paper 9c: Machine Learning the Thermochemistry of All Inorganic Crystalline Solids
— ***Christopher J. Bartel***, *Ann M. Deml, Samantha L. Millican, John R. Rumptz, William Tumas, Alan W. Weimer, Stephan Lany, Vladan Stevanovic, Charles B. Musgrave, Aaron M. Holder*

4:33 Paper 9d: Designing Dopant Patterns in Indium-Doped Perovskite Oxygen Carriers
— ***Christopher L. Hanselman,*** *Dominic Alfonso, Jonathan W. Lekse, De Nyago Tafen, Christopher Matranga, David C. Miller, Chrysanthos E. Gounaris*

4:54 Paper 9e: On the Diversity of Nanoporous Materials Genome
— ***Yongjin Lee***, *Peter Boyd, Berend Smit*

5:15 Paper 9f: In-Silico Structural Analyses of Borosilicate, Aluminosilicate, and Gallosilicate Zeolites Using Effective Tetrahedral Descriptors — ***Koki Muraoka***, *Tatsuya Okubo, Watcharop Chaikittisilp*

5:36 Paper 9g: Computational Identification of Hetero-Interpenetrated Porous Materials — ***Jihan Kim***, *Ohmin Kwon, Sanghoon Park*

(10) Advances in Algae-Based Biorefineries: Algae Biomass Cultivation, Harvesting, and Characterization
Sunday, Oct 29, 3:30 PM
MCC, 200D

Bo Hu, Chair
Robert Gardner, Co-Chair

Sponsored by:
Biorefinery Technologies for Forest-Based Lignocellulosic Biomass

3:30 Paper 10a: Bioprocess Model and Economic Analysis of Microalgae Production in Flat-Panel Photobioreactors Taking into Account Geospatial Factors
— ***Sudhanya Banerjee***, *Shri Ramaswamy*

3:50 Paper 10b: Continuous Photobioreactor Cultivation of *Nannochloropsis oculata* to Isolate Cosmetic-Grade Phospholipids
— ***Ahmet Y. Manisali***, *Ioannis Dogaris, George Philippidis, Aydin K. Sunol*

4:10 Paper 10c: Effects of pH on Cell Growth, Lipid Production and CO_2 Demand of Microalgae *Chlorella sorokiniana* — ***Renhe Qiu***, *Kimberly Ogden*

4:30 Paper 10d: Microalgae Fractionation and Recovery of Native Components Through Application of Low-Cost Enzymes
— ***Godwin Abel***, *Heng Shao, Agasteswar Vadlamani, Patricia Relue, Sridhar Viamajala, Sasidhar Varanasi*

4:50 Paper 10e: Design of Marine Macroalgae Photobioreactor Integrated into Building with Natural Sun Illumination
— ***Alexander Golberg***, *Alexander Chemodanov, Arthur Robin*

5:10 Paper 10f: An Integrated Approach for Bioenergy Production from Microalgae Using Solar Energy, CO_2 and Wastewater — ***Nasir Al Lagtah***

(11) Advances in Industrial Reaction Engineering and Catalysis
Sunday, Oct 29, 3:30 PM
MCC, 102D

Jan J. Lerou, Chair
Carmo Pereira, Co-Chair
Concetta La Marca, Co-Chair
Marc-Olivier Coppens, Co-Chair
Sagar Sarsani, Co-Chair
Andrew Teixeria, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

3:30 Paper 11a: Insight into the Formation Mechanism of an Industrially Relevant Ziegler–Natta Catalyst
— ***Antoine Klaue***, *Hua Wu, Massimo Morbidelli, Matthias Kruck, Nicolaas Friederichs, Francesco Bertola*

3:51 Paper 11b: Use of Sacrificial Agent to Enhance Gas Transport Through the Washcoat
— ***Pritpal Singh Dhillon***, *Michael Harold, Di Wang, Ashok Kumar*

4:12 Paper 11c: Bifurcation Analysis of Gas-Phase Methane Oxidative Coupling
— ***Zhe Sun***, *Arun Kota, Sagar Sarsani, David H. West, Vemuri Balakotaiah*

4:33 Paper 11d: Nanoengineering the Environment Around Catalytic Active Sites
— ***Michael M. Nigra***, *Nidhi Kapil, Marc-Olivier Coppens*

4:54 Paper 11e: Fabrication of Ultra-Thin PVP-Metal Oxide Nanofibers via Electrospinning for Applications in Catalysis and Adsorption
— ***Faisal H. Alshafei***, *Sara Azzam, Luke Minardi, Derrick Rosales, Dante Simonetti*

5:15 Paper 11f: Microfluidic Studies of Room-Temperature Synthesized Perovskite Nanocrystals
— ***Milad Abolhasani***

5:36 Paper 11g: Ultrafast Synthesis of Titanium Silica(TS-1) by Continuous Flow
— ***Yunpeng Hu***, *Kai Wang, Tao Wang Sr., Guangsheng Luo*

(12) Advances in Process Control
Sunday, Oct 29, 3:30 PM
MCC, 103E

Fernando V. Lima, Chair
Ravendra Singh, Co-Chair

Sponsored by:
Systems and Process Control

3:30 Paper 12a: Accounting for Safety System Activation Within Economic Model Predictive Control
— ***Fahad Albalawi***, *Zhe Wu, Zhihao Zhang, Helen Durand, Panagiotis D. Christofides*

3:49 Paper 12b: A Novel Biomimetic Approach to Process Control by Exploiting Memory and Cognition
— ***Jacob Albright***, *Debangsu Bhattacharyya*

4:08 Paper 12c: Control with Soft Feedback in Social Systems: Mathematical Principles, Empirical Evidence, and Applications
— ***Yu Luo***, *Garud Iyengar, Venkat Venkatasubramanian*

4:27 Paper 12d: A Novel, Biomimetic Approach to Self-Organizing, Optimal Control Structure Design
— ***Temitayo Bankole***, *Debangsu Bhattacharyya, Berhane Gebreslassie, Urmila M. Diwekar*

4:46 Paper 12e: Closed-Loop Active Fault Diagnosis for Uncertain Nonlinear Systems
— ***Joel Paulson***, *Tor Aksel N. Heirung, Marc Martin-Casas, Ali Mesbah*

5:05 Paper 12f: Development of a Biologically Inspired Approach for Advanced Adaptive Control of Clean Energy Systems
— ***Gaurav V. Mirlekar***, *Ghassan Al-Sinbol, Mario Perhinschi, Fernando V. Lima*

5:24 Paper 12g: A New Dynamic-Response Surface Methodology for Modeling the Dynamics of Nonlinear Processes
— ***Zhenyu Wang***, *Christos Georgakis*

5:43 Paper 12h: The Stabilization of Input-Constrained Nonlinear Systems with Maximal Region of Attraction
— ***Tyler Homer***, *Prashant Mhaskar*

(13) Agglomeration and Granulation Processes
Sunday, Oct 29, 3:30 PM
MCC, 200H

Jim Michaels, Chair
Mehrdad Kheiripour, Co-Chair

Sponsored by:
Particle Production and Characterization

3:30 Paper 13a: Surface Velocity Measurements of a Powder Bed in a High-Shear Wet Granulator Using High-Speed Video Analysis
— ***Patrick Wray***, *John Jones, Peter Ferrie, Jay Poorna Reddy, Preetanshu Pandey, Stuart Charlton, Andrew Dennis*

3:49 Paper 13b: Development of an Inline Measurement Tool for Particle Size and Shape Analysis During the Granulation Process
— ***Maria Niesing,*** *Dominik Weis, Sergiy Antonyuk, Markus Thommes*

4:08 Paper 13c: Single-Drop Impact on Heterogeneous Powder Beds Through Granule Formation Mechanisms, Drop Penetration Time, and Granule Morphology and Structure
— ***Tianxiang Gao***, *Arun Sundar S. Singaravelu, Nikhilesh Chawla, Heather N. Emady*

4:27 Paper 13d: DEM Investigation on the Dynamics of Singlet-Doublet Collisions of Cohesive Particles
— ***Peiyuan Liu,*** *Kevin M. Kellogg, Casey Q. LaMarche, Christine M. Hrenya*

4:46 Paper 13e: Interval Type-2 Fuzzy Predictive Modelling for a High-Shear Granulation Process
— ***Wafa' H. AlAlaween***, *Mahdi Mahfouf, Agba Salman*

5:05 Paper 13f: Experimental Investigation and Modelling of the Deformation Behavior of Pharmaceutical Pellets as a Basis for DEM Simulations of the Spheronization Process
— ***Dominik Weis***, *Maria Niesing, Markus Thommes, Sergiy Antonyuk*

5:24 Paper 13g: A Mechanistic Model for Granule Breakage in Twin-Screw Granulation
— ***Shankali U. Pradhan***, *Jiayu Li, James D. Litster, Carl R. Wassgren*

5:43 Paper 13h: Experimental Investigation of a Dry Slag Granulation Unit Using a Rotating Disc
— ***P. C. Seshasai***, *Y. Eswararao, S. Pushpavanam, T. Renganathan*

(14) Amorphous Solid Dispersions for Drug Product
Sunday, Oct 29, 3:30 PM
MCC, 205A/B

Justin D. Moser, Chair
Anil Rane, Co-Chair

Sponsored by:
Pharmaceutical Discovery, Development and Manufacturing Forum

3:30 Paper 14a: Sustained Supersaturation of Erlotinib SDD Ternary Amorphous Systems
— ***Kimberly B. Shepard***, *Michael Morgen*

3:50 Paper 14b: Connecting the Product-Process-Performance Interplay for Improved Understanding in Development of a Spray-Dried Dispersion Drug Product
— ***Justin D. Moser***, *Jesse Kuiper*

4:10 Paper 14c: Strategically Designed Polymer Synthons as Pharmaceutical Excipients in Oral Drug Delivery
— ***Jeffrey Ting***, *Swapnil Tale, Anatolii Purchel, Seamus D. Jones, Monica Ohnsorg, Soroush Moghadam, Li Guo, Steven Guillaudeu, Ronald G. Larson, Frank S. Bates, Theresa M. Reineke*

4:30 Paper 14d: Pill Burden Reduction Through Engineering the Mechanical Properties of Spray-Dried Amorphous Solid Dispersions — ***Alyssa Ekdahl***, *Aaron Goodwin, Deanna Mudie*

4:50 Paper 14e: Reprocessing of Spray-Dried Dispersions: Minimizing Resources in Process Development and Dealing with the Possible Failure
— ***Tiago Porfirio***, *Íris Duarte, Rui Ferreira, Bruno Henriques, João Vicente, Viriato Semião*

5:10 Paper 14f: In-Silico Development of Amorphous Solid Dispersions for Optimal Performance and Stability
— ***Pedro Valente***, *Íris Duarte, Márcio Temtem*

5:30 Paper 14g: Experimental and Model-Based Optimization of a Secondary Drying Process for a Spray-Dried Dispersion Product
— ***Li Tan***, *Christoph Gesenberg, Joshua Engstrom, Jason Sweeney*

(15) Biobased Fuels and Chemicals: Biosynthetic Pathway Engineering & Enzymatic Conversion
Sunday, Oct 29, 3:30 PM
MCC, 208C/D

Jose L. Avalos, Chair
Cong T. Trinh, Co-Chair

Sponsored by: Bioengineering

3:30 Paper 15a: Identification and Reconstruction of Pathways for Lignin Catabolism
— ***Joshua K. Michener***

3:48 Paper 15b: Investigating New Pathways and a 'Funneling' Strategy to Enhance Production of Chemicals Derived from Shikimic Acid Biosynthesis
— *Brian Thompson, Shawn Pugh, Michael Machas,* ***David R. Nielsen***

4:06 Paper 15c: Engineering of ADP1 for Production of Vanillin from Lignin
— ***Shu Huang***, *Bradley W. Biggs, Keith E. J. Tyo*

4:24 Paper 15d: C_4-C_9 Alcohols Production by '+1' Pathway-Engineered *E. coli:* Evaluation of Vector Expression Systems and Fermentation Process Conditions
— ***Mamatha Devarapalli***, *Paresh Sanghani, Chris Stowers, Sarah Delaplane, Ryan Hill, Devon Rosenfeld*

4:42 Paper 15e: Establishing a Platform *Escherichia coli* Strain to Generate Xylose-Derived Value-Added Products
— ***Jia Wang***, *Xiaolin Shen, Qipeng Yuan, Yajun Yan*

5:00 Paper 15f: Understanding and Enhancing Bioconversion of Acetic Acid to Biodiesel Using *Yarrowia lipolytica*
— ***Nian Liu***, *Kangjian Qiao, Junyoung O. Park, Zbigniew Lazar, Gregory N. Stephanopoulos*

5:18 Paper 15g: Metabolic Engineering of Bacteria for Production of Oleochemicals
— ***Brian F. Pfleger***

(16) Biomaterials for Nucleic Acid Delivery
Sunday, Oct 29, 3:30 PM
MCC, 211C

Millicent Sullivan, Chair
John Wilson, Co-Chair
Christopher A. Alabi, Co-Chair

Sponsored by: Biomaterials

3:30 Paper 16a: Lipid-Like Materials for RNA Delivery: A How-To Guide for Hacking Gene Expression
— ***Kathryn A. Whitehead***

4:06 Paper 16b: Triple Delivery Nanoscale Device for siRNA, Vismodegib and Gemcitabine Co-Delivery to Treat Pancreatic Cancer
— ***Metin Uz***, *Satyanarayana Rachagani, Surinder Batra, Surya K. Mallapragada*

4:24 Paper 16c: Influence of Dextran and Surface Charge on Nanoparticle-Mediated siRNA Delivery
— ***Daniel Vocelle***, *Olivia Chesniak, Mitch Smith, Christina Chan, S. Patrick Walton*

4:42 Paper 16d: PEG-Poly (beta-amino ester) Delivery Systems for Periodic shRNA
— ***Connie Wu***, *Jiahe Li, Wade Wang, Paula T. Hammond*

5:00 Paper 16e: Structurally Programmed Assembly of Ribonucleoproteins for Superior mRNA Delivery
— ***Jiahe Li,*** *Wade Wang, Yanpu He, Yingzhong Li, Darrell J. Irvine, Paula T. Hammond*

5:18 Paper 16f: Cationic Peptide Amphiphile Micelles (PAMs) as Nucleic Acid-Based Adjuvants Carriers for the Improvement of Subunit Vaccine Efficiency
— ***Rui Zhang***, *Josiah Smith, Jake Kramer, Logan Morton, Brittany Allen, Caitlin Leeper, Xiaolei Li, Fabio Gallazzi, Tommi White, Bret Ulery*

(17) Bionanotechnology for Gene and Drug Delivery I
Sunday, Oct 29, 3:30 PM
MCC, 212A/B

Joo Youp Lee, Chair
Elizabeth Nance, Co-Chair
Yoonjee Park, Co-Chair
Aaron C. Anselmo, Co-Chair

Sponsored by: Bionanotechnology

3:30 Paper 17a: Core Crosslinked Nanoparticles for Treating Traumatic Brain Injury
— ***Forrest Kievit***, *Christine Yoo, Abby M. Kelly, Alexander Magsam, Patrick S. Stayton, Anthony J. Convertine*

3:45 Paper 17b: Targeted Polyanhydride Nanoparticles to Combat Neurodegeneration
— ***Benjamin Schlichtmann***, *Shivani Ghaisas, Vellareddy Anantharam, Anumantha Kanthasamy, Surya Mallapragada, Balaji Narasimhan*

4:00 Paper 17c: ssDNA Nanotubes Targeting Glioblastoma Multiforme
— ***Michael A. Harris***, *Maple Shiao, Huihui Kuang, Walter C. Low, Efrosini Kokkoli*

4:15 Paper 17d: Enzyme-Encapsulating Polymeric Nanoparticles for Treating Glutamate Excitotoxicity
— ***Rick Liao***, *Catherine Panlilio, Belinda Garana, Elizabeth Nance*

4:30 Paper 17e: Design of Self-Assembled Nanostructures Built from Immune Signals to Combat Autoimmune Disease
— ***Lisa Tostanoski***, *Christopher M. Jewell*

4:45 Paper 17f: siRNA-Loaded Lipidoid Nanoparticles for Diabetic Ulcer Treatment
— ***Lisa Kasiewicz,*** *Kathryn A. Whitehead*

5:00 Paper 17g: Folic Acid-Stabilized Copper Metal-Organic Frameworks Improve Wound Healing in Diabetes
— ***Guillermo Ameer***

5:15 Paper 17h: Sequential Co-Delivery of EGFR Inhibitor and Doxorubicin for Targeted Combination Chemotherapy
— ***Zilan Zhou***, *Joo-Youp Lee, Mina Jafari*

(18) Bioseparations and Downstream Processing
Sunday, Oct 29, 3:30 PM
MCC, 206A/B

Dimple Kundiyana, Chair
Seongkyu Yoon, Co-Chair

Sponsored by: Bioengineering

3:30 Paper 18a: Addressing the Downstream Challenges of Viral Therapy for Cancer Treatment: A Study of Rhabdoviral Vector Purification
— ***Shabnam Shoaebargh***, *Vitaliya Bardal, Maria Fe Medina, Adam Smith, Joris Van der Heijden, John Bell, Brian Lichty, David R. Latulippe*

3:48 Paper 18b: A Small-Molecule-Based Affinity Membrane Spin Column for Antibody Purification
— ***Nur Mustafaoglu***, *Michael Canonico, Franklin Mejia, Basar Bilgicer*

4:06 Paper 18c: Removal of Cyanobacterial Toxins Using Polymeric Nanoparticles
— *Mousumi Bose,* ***Sutapa Barua***

4:24 Paper 18d: Increased Production of Yersiniabactin (Ybt) and the Anthranilate Analog Through Media Optimization and Ybt Metal Binding Characterization
— ***Nicholas Moscatello***, *Ruiquan Qi, Blaine Pfeifer*

4:42 Paper 18e: Applications of Magnetically Responsive Micro/Mesoporous Carbon Adsorbents in Biorefining
— *Kyle Staggs, Zhe Qiang, Andrew Flores, Xuan Wang, Bryan D. Vogt,* ***David R. Nielsen***

5:00 Paper 18f: Improving Enzymatic Synthesis of β-Lactam Antibiotics by In-Situ Crystallization
— ***Matthew A. McDonald***, *Lukas Bromig, Andreas S. Bommarius, Martha A. Grover, Ronald W. Rousseau*

5:18 Paper 18g: Separation of Fatty Acids and Fatty Acid Esters Using Nanoporous Polymeric Membranes
— ***Ned B. Bowden***, *Chad Gilmer*

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(19) CAST Director's Student Presentation Award Finalists
Sunday, Oct 29, 3:30 PM
MCC, 103D

Mario Richard Eden, Chair
Michael Nikolaou, Co-Chair

Sponsored by:
Computing Systems and Technology Division

3:30 Paper 19a: Optimal Planning of Electric Power Infrastructures
— ***Cristiana L. Lara,***
Ignacio Grossmann

3:49 Paper 19b: SPICE: A Computer-Aided Framework for Systematic Process Intensification of Chemical Enterprises
— ***Jianping Li***, Salih E. Demirel, Akhil Arora, M. M. Faruque Hasan

4:08 Paper 19c: Distributed Output-Feedback Fault Detection and Isolation of Cascade Process Networks
— ***Xunyuan Yin***, *Jinfeng Liu*

4:27 Paper 19d: A Branch-and-Bound Scheme for K-Adaptability Problems in Robust Optimization
— ***Anirudh Subramanyam***, Wolfram Wiesemann, Chrysanthos E. Gounaris

4:46 Paper 19e: A Novel Noncooperative Modeling Framework for Economic and Environmental Life-Cycle Optimization of Supply Chains and Product Systems: MIBLP Model and Efficient Solution Algorithm
— ***Jiyao Gao***, Fengqi You

5:05 Paper 19f: A Sequential Approach to Global Flowsheet Optimization Using McCormick Relaxations
— ***Dominik Bongartz***, Alexander Mitsos

5:24 Paper 19g: Semi-Supervised Anomaly Detection for Production Oil Wells
— ***Kristen Severson***, *Paphonwit Chaiwatanodom, Mark Molaro, Richard D. Braatz*

5:43 Paper 19h: A Critical Comparison of Stochastic and Worst-Case Robust Approaches to Optimal Experiment Design
— ***Marc Martin-Casas***, Dries Telen, Philippe Nimmegeers, Jan Van Impe, Ali Mesbah

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(20) Cells, Organs, and Labs on a Chip
Sunday, Oct 29, 3:30 PM
MCC, 208B

Jeremiah J. Zartman, Chair
Umut Gurkan, Co-Chair
Yaakov Nahmias, Co-Chair

Sponsored by:
Engineering Fundamentals in Life Science

3:30 Paper 20a: A Microfluidic Model of Hemostasis Sensitive to Platelet Function and Coagulation
— *Rogier M. Schoeman, Nicholas Danes, Karin Leiderman, Keith B. Neeves,* ***Matthew Sorrells***

3:48 Paper 20b: Microfluidic Platforms for Aging Studies
— ***Sahand Saberi Bosari***, *Daniel Midkiff, Adriana San-Miguel*

4:06 Paper 20c: Microfluidic Platform to Decode Mechanotransduction Mechanisms in Developing Organs
— *Cody Narciso, Nicholas Contento, Thomas Storey, David Hoelzle,* ***Jeremiah J. Zartman***

4:24 Paper 20d: 3D Biomimetic Model for Cellular Invasion: A Versatile Platform to Examine 3D Physiological Invasion in Angiogenesis and Pathological Tumor Cell Invasion
— ***Duc-Huy Nguyen***, *Sina Rabbany, Robert Schwartz, Shahin Rafii*

4:42 Paper 20e: "Lymphatics-on-a-Chip" to Reconstitute Lymphatic Drainage Function and Lymphedema
— ***Esak Lee***, *Christopher Chen*

5:00 Paper 20f: An Optically Controlled Microphysiological System for the Heart-Brain Axis
— *Jonathan Soucy, Tess Torregrosa, Abigail Koppes, Nasim Annabi,* ***Ryan Koppes***

5:18 Paper 20g: Contracting 3D-Printed Microtissues: Solid and Fluid Instabilities — ***Thomas Angelini***

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(21) Characterization and Measurement in Powder Processing
Sunday, Oct 29, 3:30 PM
MCC, 200I

Bodhisattwa Chaudhuri, Chair
Michael Winn, Co-Chair

Sponsored by:
Solids Flow, Handling and Processing

3:30 Paper 21a: Applying Inline Spatial Filter Velocimetry to Improve Process Robustness of a Continuous Twin-Screw Wet Granulator
— ***Niels Nicolaï***, *Ingmar Nopens, Krist V. Gernaey, Thomas De Beer*

3:49 Paper 21b: The Use of Flow Aids to Prevent Caking of Bulk Solid Materials — ***Kerry Johanson***

4:08 Paper 21c: Novel Starch-Salt Composites: Their Strength, Composition and Scale-Up Investigated and Characterized
— ***Gabrie Meesters***, *Vincent Jansen, Dorine Hugenholz, Chengda Pan, Robbert Dijkhuizen, Henk Nugteren*

4:27 Paper 21d: Derivative Peak Fitting of Differential Diffuse Reflectance for Compositional Analysis of Multiphase Semiconductor, P25 TiO_2
— ***Ashley M. Pennington***, *George Tsilomelekis, Fuat E. Celik*

4:46 Paper 21e: Real-Time, In-Line Assessment of Flow Performance for Compressible and Anisotropic Bulk Solids — ***Tyler L. Westover***, *Glen Monson, Sergio Hernandez, Jordan Klinger, Kunal Pardikar, Carl R. Wassgren*

5:05 Paper 21f: Drag Force Flow Sensors for In-Line Monitoring of Powder Processes
— ***Thom Freeman***, *John Yin, Katrina Brockbank*

5:24 Paper 21g: Surface Energy and Its Effect on Interparticle Interaction During Particle Flow
— ***Camila Garcia Jange***, *Rose Prabin Kingsly Ambrose*

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(22) Cutting-Edge and Innovative Corporate & Industrial Research Projects (Invited Talks)
Sunday, Oct 29, 3:30 PM
MCC, 101H

Victoria Baldwin, Chair
Noah D. Meeks, Co-Chair

Sponsored by:
Young Professionals Committee (YPC)

3:30 Paper 22a: Predicting Temperature-mediated Solid Form Transformations in Small Molecule Crystals with Molecular Dynamics
— ***Eric Dybeck***

3:55 Paper 22b: Polymer D-255 Cement Fluid Loss Additive Control Optimization — ***AnnaLaura Arredondo***

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(23) Engineering the Tissue and Cell Microenvironment
Sunday, Oct 29, 3:30 PM
MCC, 208A

Julianne L. Holloway, Chair
Gargi Ghosh, Co-Chair
Ethan S. Lippmann, Co-Chair

Sponsored by:
Engineering Fundamentals in Life Science

3:30 Paper 23a: Adaptable Biomaterials to Maintain Stemness of Neural Progenitor Cells
— *Christopher M. Madl,* ***Sarah C. Heilshorn***

4:10 Paper 23b: Radiation-Induced Changes in the Extracellular Matrix Alter the Invasiveness of Heterogeneous Tumors
— ***Marjan Rafat***, *Ninna Rossen, Hussein Shehade, Katrina Wisdom, Janine Erler, Amato J. Giaccia, Edward E. Graves*

4:28 Paper 23c: A 3D Bicellular Biomimetic Model of Vasculitis Reveals New Insights into Vascular Barrier Function
— ***Stella Alimperti***, *Teodelinda Mirabella, Varnica Bajaj, William Polacheck, Jeroen Eyckams, Christopher Chen*

4:46 Paper 23d: Rapid Generation and Simultaneous Detection of Biomimetic Oxygen Concentration Gradients In Vitro
— ***Md. Daud H. Khan***, *Steven Roberts, John Robert Cressman, Nitin Agrawal*

5:04 Paper 23e: Evaluation of a Chitosan-Gelatin Thermogelling Hydrogel as a Bioprinter Ink Using an Inexpensive Platform
— ***Kevin D. Roehm***, *Sundararajan V. Madihally*

5:22 Paper 23f: Engineered Peptide-Modified Hydrogel Platform for Biomanufacturing of Human Pluripotent Stem Cells
— ***Thomas Richardson***, *Fatimah Adisa, Joseph E. Candiello, Prashant N. Kumta, Ipsita Banerjee*

5:40 Paper 23g: Substrate Surface Tension and Marangoni Effects Mediate Cell-Cell Coordination in Migration and Multicellular Assembly
— ***Zhu Cheng***, *Matthew Paszek*

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(24) Green Chemical Reaction Engineering for Sustainability
Sunday, Oct 29, 3:30 PM
MCC, 103A

Samuel Marre, Chair
Simon Kuhn, Co-Chair
Ali A. Rownaghi, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

3:30 Paper 24a: Nitrogen Recovery and Biocrude Formation from Hydrothermal Liquefaction of Protein
— ***James Sheehan***, *Phillip E. Savage*

3:50 Paper 24b: Bio-Succinic Acid Production from Tartaric Acid
— ***Jiayi Fu***, *Efterpi Vasiliadou, Basudeb Saha, Dionisios G. Vlachos*

4:10 Paper 24c: 1,6-Hexanediol Synthesis from Cellulose
— ***Jiayue He***, *Samuel P. Burt, Kevin J. Barnett, Siddarth H. Krishna, Kefeng Huang, David Martin Alonso, Madelyn Ball, Christos T. Maravelias, Ive Hermans, James Dumesic, George W. Huber*

4:30 Paper 24d: High-Efficiency Photo-Electrochemical Chloro-Alkali Production
— ***Miguel Modestino***, *Demetri Psaltis, Christophe Moser, Enrico Chinello, Laurent Coulot, Mathieu Ackermann, Florian Gerlich*

4:50 Paper 24e: Gold Nanoparticle Catalysis: Colloidal Versus Supported Heterogeneous Catalysis and Methods for Colloidal Nanoparticle Recovery
— ***Saptarshi Chakraborty***, *Siyam Ansar, Jennings Stroud, Christopher L. Kitchens*

5:10 Paper 24f: Isosorbide Production from Aqueous Sorbitol Solution over Silica-Aluminas
— ***Thanh Khoa Phung***, *Md. Anwar Hossain, Teerawit Prasomsri, Noppadon Sathitsuksanoh*

5:30 Paper 24g: Simple One-Step Reaction to Achieve Cross-Linked Polymer and Polymer Composites: Models for Rubber Tires That Can Be Recycled Multiple Times with Robust Recovery of Properties Related to Cross-Link Density
— ***John M. Torkelson***, *Kailong Jin, Lingqiao Li*

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(25) Green Chemistry and Engineering
Sunday, Oct 29, 3:30 PM
MCC, 101D

Donna Bryant, Chair
Marimuthu Andiappan, Co-Chair

Sponsored by: General

3:30 Paper 25a: Bio/Catalytic Synthesis of Methacrylic Acid
— ***Maryam Pirmoradi***, *James Kastner*

3:51 Paper 25b: Nitrogen-Efficient Fertilizer Design Based on Urea Adducts — ***Jonas Baltrusaitis***

4:12 Paper 25c: Green Processes to Use Extract from Citrus Peel Waste for Novel Applications (Direct Polystyrene Recycling to Natural Solvent to Source of Carbon)
— *Shital Yadav,* ***Chandra S. Sharma***

4:33 Paper 25d: Development and Applications of Profitable Pollution Prevention Technologies
— ***Helen Lou***, *Yinlun Huang*

4:54 Paper 25e: Kinetics, Yield and Rate-Limiting Processes in the Biosynthesis of Colloidal Silver Nanoparticles by a Fresh Water Microalga
— ***Ashiqur Rahman***, *Shishir V. Kumar, Tsai-Nan Mai, Adarsh Bafana, Prasad P. Pawar, Si A. Dahoumane, Clayton S. Jeffryes*

5:15 Paper 25f: Microwave-Assisted Synthesis of Silver Nanoparticles Using Glucose and Starch
— ***Shishir V. Kumar***, *Adarsh Bafana, Prasad P. Pawar, Ashiqur Rahman, Si A. Dahoumane, Clayton S. Jeffryes*

5:36 Paper 25g: Enhancing Energy Efficiency in Saccharide-HMF Conversion with Core/Shell-Structured Microwave-Responsive Catalysts
— ***Tuo Ji***, *Jiahua Zhu*

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(26) Green Pharmaceutical Process Development and Biocatalysis
Sunday, Oct 29, 3:30 PM
MCC, 204A/B

Andreas S. Bommarius, Chair
Shane T. Grosser, Co-Chair

Sponsored by:
Pharmaceutical Discovery, Development and Manufacturing Forum

3:30 Paper 26a: Developing Improved Enzymes for Industrial Biocatalysis
— ***Iman Farasat***

3:55 Paper 26b: Technoeconomic Optimisation, Antisolvent Selection and Comparative Environmental Evaluation for Continuous Paracetamol Crystallisation
— ***Hikaru G. Jolliffe***, *Dimitrios I. Gerogiorgis*

4:20 Paper 26c: Metric-Driven Process Development of a Late-Stage Drug Substance
— ***Kathleen Lauser***, *Nathan Domagalski, Michaël Fenster, Thomas La Cruz, Max A. Mellmer, Eric M. Saurer, Matthew Winston*

4:45 Paper 26d: Scalable Continuous Synthesis of Enantiomerically Pure Amine APIs in an Enzyme Membrane Reactor
— ***Robert D. Franklin***, *Bettina Bommarius, Andreas S. Bommarius*

5:10 Paper 26e: Development of a Biocatalytic Cascade for the Deracemization of a Racemic Alcohol
— ***Shane T. Grosser***

5:35 Paper 26f: Design of New Reactors to Produce Levan Biopolymer Through Enzymatic Catalysis: Kinetics and Mass Transfer
— ***Álvaro González-Garcinuño***, *Alvaro Sanchez, Sonia Ruiz, Antonio Tabernero, Miguel A. Galan, Montaña Elviro, Antonio Monzón,* ***Eva Martín del Valle***

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(27) In Honor of Dennis Prieve's Retirement I (Invited Talks)
Sunday, Oct 29, 3:30 PM
MCC, 101A

Christopher L. Wirth, Chair
Jeffrey A. Fagan, Co-Chair
Robert D. Tilton, Co-Chair

Sponsored by: Interfacial Phenomena

3:30 Welcoming Remarks

3:33 Paper 27a: Anisotropic Particle Interactions with Surfaces, Other Particles, and External Fields
— ***Michael A. Bevan***

3:51 Paper 27b: Particle-Wavy Wall Interactions in a Nematic Liquid Crystal
— ***Kathleen Stebe***, *Yimin Luo, Francesca Serra*

4:09 Paper 27c: Influence of Surface Roughness on Particle-Substrate Interactions: Double Layer Repulsion, Van Der Waals Attraction, and Depletion Interaction
— ***Sven H. Behrens***, *Joanna W. Tsao*

4:27 Paper 27d: Functional Particles and Microcapsules
— ***Simon Biggs***, *Alison Tasker*

4:45 Paper 27e: The Hindered Translational and Rotational Dynamics of Anisotropic Nanoparticles Diffusing near a Solid-Liquid Interface Measured in Aqueous Solution
— ***Christopher Bolton***, *Raymond R. Dagastine*

5:03 Paper 27f: Strong Deformation of the Electric Double Layer During Sedimentation or Electrophoresis of a Charged Particle — ***Aditya S. Khair***

5:21 Paper 27g: Understanding and Engineering Diffusiophoretic Suspensions — ***Todd M. Squires***

5:39 Paper 27h: Chemically Driven Transport: A Pervasive Mechanism That Is Seldom Recognized
— ***Darrell Velegol***

5:57 Concluding Remarks

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(28) Life-Cycle Analysis of Bio-Based Fuels, Energy, and Chemicals
Sunday, Oct 29, 3:30 PM
MCC, 101B

David R. Shonnard, Chair
Yuan Yao, Co-Chair

Sponsored by:
Sustainable Biorefineries

3:30 Paper 28a: Impacts of CO_2 Supply Systems for Algal-Based Biorefineries on Biofuel Life-Cycle Assessments
— ***Matthew J. Realff***, *Ronald R. Chance, Teresa Fishbeck, Howard Hendrix, Valerie Thomas, Sathvik Varma, Yanhui Yuan*

3:55 Paper 28b: Carbon Fixation by RuBisCo-Nanostructure Complex to Produce 3-Phosphoglyceric Acid: A Life-Cycle Assessment
— ***Kyuha Lee***, *Yuan Sun, Jon R. Parquette, Bhavik R. Bakshi*

4:20 Paper 28c: Life-Cycle Assessment of Biofuel and Bioenergy Production from Brown Algae Through Biochemical Pathways
— ***Peyman Fasahati***, *Christopher M. Saffron, J. Jay Liu*

4:45 Paper 28d: Integrated Design and Analysis of Chemical Production from Biomass Feedstocks
— ***Abhay Athaley***, *Praneeth Annam, Basudeb Saha, Marianthi Ierapetritou*

5:10 Paper 28e: Life-Cycle Analysis (LCA) of Bio-Derived Terephthalic Acid (TPA) and Bio-Derived-Hexamethylenediamine (HMDA)
— ***Pahola Thathiana Benavides***, *Jennifer B. Dunn, Jeongwoo Han, Mary Biddy*

5:35 Paper 28f: Sustainability Analysis of Condensed-Phase n-Butanol Production from Ethanol
— ***Iman Nezam***, *Christopher M. Saffron, Andrew Juergens, Michal Mulik, Eric Wiitanen, Dennis J. Miller*

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(29) Liquid-Phase Reaction Engineering
Sunday, Oct 29, 3:30 PM
MCC, 102E

Daniel Chen, Chair
Joris W. Thybaut, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

3:30 Paper 29a: Selective Liquid-Phase Hydrogenation of Chloronitrobenzene over AuPd Nanoclusters on TiO_2 Catalysts
— ***Yu-Wen Chen***

3:52 Paper 29b: Process Intensification for the Aqueous-Phase Dehydration of Biomass-Derived Carbohydrates
— ***Pierre Desir***, *Basudeb Saha, Dion Vlachos*

4:14 Paper 29c: Organocatalyzed Beckmann Rearrangement of Cyclohexanone Oxime in a Microreactor: Kinetic Model and Product Inhibition
— ***Chencan Du***, *Jisong Zhang, Guangsheng Luo*

4:36 Paper 29d: Modeling the Influence of Dean Vortices in Improving the Performance of Catalytic Membrane Microreactors
— ***A. Choudhary***, *S. Pushpavanam*

4:58 Paper 29e: Enhancing Reaction Rates by Automated In-Silico Solvent Screening — ***Christoph U. Gertig***, *Leif C. Kröger, Jan D. Scheffczyk, Jens Langanke, Kai Leonhard, André Bardow*

5:20 Paper 29f: Enhancement of the Activity and Selectivity of the Fischer-Tropsch Synthesis with Water/Oil Emulsions
— ***Felipe Anaya***, *Daniel E. Resasco*

5:42 Paper 29g: Comparison Between Thermal- and Electro-Catalytic Upgrading of Furanic Compounds in the Liquid Phase: A Combined Experimental and DFT Study — ***Reda Bababrik***, *Bin Wang, Daniel Resasco*

(30) Materials Innovations Inspired by Acrivos Award Winner Chris Jones I
Monday, Oct 30, 8:00 AM
MCC, 211A

Nicholas Brunelli, Chair
Jason C. Hicks, Co-Chair

Sponsored by:
Materials Engineering and Sciences Division

8:00 Paper 30a: Design of Aminopolymer Structure to Enhance Performance and Stability of CO_2 Sorbents: Poly(propyleneimine) vs. Poly(ethylenimine)
— ***Simon H. Pang***, *Ryan P. Lively, Christopher W. Jones*

8:19 Paper 30b: Development of 3D-Printed Aminosilica Monoliths for CO_2 capture
— *Harshul Thakkar, Stephen Eastman,* ***Fateme Rezaei***

8:38 Paper 30c: Engineering-Supported Amine Adsorbents for CO_2 Capture Applications
— *Zelong Xie, Christopher Cogswell,* ***Sunho Choi***

8:57 Paper 30d: Impacts of Aminopolymer-Support Interaction on CO_2 Sorption Performance Probed by Neutron Scattering Techniques
— ***Adam Holewinski***, *Miles Sakwa-Novak, Matthew Potter, Nathan Ellebracht, Gernot Rother, Christopher W. Jones*

9:16 Paper 30e: Hierarchically Structured Porous Materials for Enhanced Greenhouse Gas Capture
— ***Tae-Hyun Bae***

9:35 Paper 30f: Natural Gas Adsorption in SSZ-13: Equilibrium and Dynamic Properties
— ***Joshua A. Thompson***

9:54 Paper 30g: Zeolite on Demand: Design and Synthesis of Zeolites with Controlled Crystal Morphology and Location of Substituting Tetrahedral Atoms with the Aid of Theoretical Calculations
— ***Watcharop Chaikittisilp***, *Koki Muraoka, Sye Hoe Keoh, Tatsuya Okubo*

10:13 Paper 30h: Tuning Solid Acids for the Target Catalytic Reactions
— ***Jun Huang***

(31) Modeling of Biomaterials
Sunday, Oct 29, 3:30 PM
MCC, 211D

Yi He, Chair
Forrest Kievit, Co-Chair
Qing Shao, Co-Chair

Sponsored by: Biomaterials

3:30 Paper 31a: Understanding Peptide Assembly with Coarse-Grained Models Designed by Information Theory (Invited Talk)
— ***M. Scott Shell***

4:06 Paper 31b: Modeling the Oxidative Consumption of Curcumin from Controlled-Release Poly(beta amino ester) Microparticles in the Presence of a Free Radical–Generating System
— ***Carolyn T. Jordan***, *J. Zach Hilt, Thomas D. Dziubla*

4:24 Paper 31c: The Fusion and Spreading of Liposome with Different Sizes: Molecular Dynamics Simulation with Dry-Martini Force Field
— ***Yanfei Lu***, *Lu Diannan*

4:42 Paper 31d: Design of Membrane-Embedded Amphiphilic Nanoparticles from Multiscale Simulations
— ***Reid Van Lehn***

5:00 Paper 31e: Improvement on Self-Assembly of Virus-Like Particles by the Introduction of Electrostatic Attraction
— ***Lin Zhang***, *Xiaocui Guo, Yan Sun*

5:18 Paper 31f: Contemporary Modeling and Analysis of Human Blood Rheology
— ***Matthew Armstrong***, *Tyler Helton, Evan Ousley, Michael Deegan*

5:36 Paper 31g: How Confinement and Hydrophobicity Affect CO_2 Diffusion from the Bulk Phase to the Active Site of Human Carbonic Anhydrase II: A Study Based on Coarse-Grained Molecular Dynamics Simulation and the Markov-State Model
— ***Gong Chen***, *Diannan Lu, Jianzhong Wu, Zheng Liu*

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(32) Multiscale Modeling
Sunday, Oct 29, 3:30 PM
MCC, 103B

Andrew J. Adamczyk, Chair
Tian Gu, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

3:30 Paper 32a: First-Principles Multiscale Modeling of CO Oxidation on Polycrystalline RuO_2 in a Fixed-Bed Reactor
— ***Jonathan E. Sutton***, *Juan Lorenzi, Jaron Krogel, Qingang Xiong, Karsten Reuter, Sebastian Matera, Sreekanth Pannala, Aditya Savara*

3:49 Paper 32b: Multiscale Averaged Models and Application to Dual-Layered Monolith Reactors
— ***Ram R. Ratnakar***, ***Rama Krishna Dadi***, *Vemuri Balakotaiah*

4:08 Paper 32c: Combined Quantum-Mechanical and Molecular-Mechanical Method for Catalyst Design on the Nu-1000 Metal-Organic Framework
— ***Xin-Ping Wu***, *Laura Gagliardi, Donald G. Truhlar*

4:27 Paper 32d: Multiscale Process Simulation by Combining CFD and Subgrid Modeling
— ***Thomas Eppinger***, *Ravindra Aglave*

4:46 Paper 32e: Multiscale CO_2 Conversion Modelling on Cu-Based Catalysts
— *Matej Huš, Drejc Kopač, Neja Strah Štefančič, Damjan Lašič Jurković, Venkata Dasireddy,* ***Blaž Likozar***

5:05 Paper 32f: Evaluation of Multiscale Models for Steam Methane Reforming in a Fixed-Bed Reactor
— ***Anthony G. Dixon***

5:24 Paper 32g: Parametric Studies of Steam Methane Reforming Using a Multiscale Reactor Model
— ***Flavio da Cruz***, *Secgin Karagoz, Vasilios Manousiouthakis*

5:43 Paper 32h: Kinetic Modelling and Optimization of Diesel Hydrotreating Process
— ***Luwen Gong***, *Nan Zhang*

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(33) Novel Materials for Environmental Applications
Sunday, Oct 29, 3:30 PM
MCC, 102C

Bihter Padak, Chair
Erdem Sasmaz, Co-Chair

Sponsored by: Air

3:30 Paper 33a: Synthesis of Graphene-Based Iron-Copper Bimetallic Nanocomposite and Its Environmental Applications
— ***Ayyaz Ahmad***, *Xuhong Guo, Yisheng Xu, Muhammad Danish*

3:50 Paper 33b: XPS Characterization of TiO_2 Photocatalytic Adsorptive Desulfurization
— *Mingyang Chi,* ***Bruce J. Tatarchuk***

4:10 Paper 33c: CO_2 Capture by Amine-Functionalized Metal-Organic Frameworks (MOFs), Graphene Oxide (GO), and MOF/GO Composites
— *Jeewan Pokhrel, Nidhika Bhoria, Theodore Tsoufis, George Romanos,* ***Georgios N. Karanikolos***

4:30 Paper 33d: CO_2-Driven Chemical-Looping Gasification on Doubly Doped Ceria
— ***Azadeh Amiri***, *Adam Sims, Kanchan Mondal*

4:50 Paper 33e: Mercury Capture from Coal-Fired Power Plant Flue Gas Using Zeolite-Based Sorbent Polymer Composite (SPC) Materials
— ***Vladimiros Nikolakis***, *Xiao-Chun Lu, Steve Hardwick, Uwe Beuscher, Franz Shelley*

5:10 Paper 33f: Chemisorption of Elemental Mercury onto $CuCl_2$-Impregnated Activated Carbon Sorbent
— ***Vishnu Sriram***, *Zhouyang Liu, Joo-Youp Lee*

5:30 Paper 33g: Experiments and Microkinetic Modelling of NO Reduction Using HC-SCR on Ag Catalyst
— *Vishnu Prasad, Anupam Abha,* ***Preeti Aghalayam***

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(34) Organic, Polymeric, and Hybrid Semiconductors
Sunday, Oct 29, 3:30 PM
MCC, 210A/B

Rizia Bardhan, Chair
Vivian Ferry, Co-Chair

Sponsored by:
Electronics and Photonics

3:30 Paper 34a: Printing Fully Stretchable Thin-Film-Transistor Array
— ***Jia Liu***, *Francisco M. Lopez, Jiechen Wang, Nathan G.-J. Wang, Jinyoung Oh, Sihong Wang, Zhenan Bao*

3:47 Paper 34b: Conjugated Macrocycles for Ultra-Sensitive Organic Photodetectors
— ***Yu Zhong***, *Boyuan Zhang, Xiaoyang Zhu, Colin Nuckolls*

4:04 Paper 34c: Connecting Crystalline Domains: Blending Conjugated Polymers of Differing Molecular Weights for Enhanced Charge Transport
— ***Michael McBride***, *Nils Persson, Danny Keane, Martha A. Grover, Elsa Reichmanis*

4:21 Paper 34d: Ultrafast Carrier Dynamics in Bimetallic Nanostructures-Enhanced Methylammonium Lead Bromide Perovskites
— ***Rizia Bardhan***

4:38 Break

4:48 Paper 34e: Aggregation Structure and Solvation of Solution-Phase PTB7
— ***Daniel Reid***, *Nicholas Jackson, Juan de Pablo*

5:05 Paper 34f: Self-Aligned Strategy for Printed Electronics
— ***Woo Jin Hyun***, *Lorraine F. Francis, C. Daniel Frisbie*

5:22 Paper 34g: Helical Perylene Diimide Ribbons for Molecular Electronics
— ***Yu Zhong***, *Michael Steigerwald, Xiaoyang Zhu, Fay Ng, Colin Nuckolls*

5:39 Paper 34h: Modulating Charge Transport in Vapor-Deposited Organic Semiconductors
— ***Nicholas Jackson***, *Lucas Antony, Juan De Pablo*

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(35) Panel Speakers Forum: Chemical Process and Product Careers in Academia vs. Industry
Sunday, Oct 29, 3:30 PM
MCC, 102B

Kishori T. Deshpande, Chair
Sitaraman Krishnan, Co-Chair
Mosha H. Zhao, Co-Chair

Sponsored by:
Process Development Division

3:30 Paper 35a: Kenneth R. Cox, Chemical and Biomolecular Engineering, Rice University, Houston, TX
— ***Kenneth R. Cox***

3:55 Paper 35b: Jean W. Tom, Chemical Development, Bristol-Myers Squibb, New Brunswick, NJ
— ***Jean W. Tom***

4:20 Paper 35c: Robert S. Huss, Eastman Chemical Company, Kingsport, TN
— ***Robert S. Huss***

4:45 Paper 35d: Tom Enright, Scale-Up Engineering, Xerox Research Center of Canada, Mississauga, Ontario, Canada
— ***Tom Enright***

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(36) Polymer Reaction Engineering
Sunday, Oct 29, 3:30 PM
MCC, 211B

Christopher J. Ellison, Chair
Narayan Ramesh, Co-Chair

Sponsored by: Polymers

3:30 Paper 36a: Engineering Pathways to New Functional Polyether Materials
— ***Nathaniel A. Lynd***

4:00 Paper 36b: Topology Control of Bottlebrush Polymers
— ***Damien Guironnet***, *Dylan Walsh*

4:15 Paper 36c: A New, Facile Approach to Epoxide Polymerization
— ***Robert C. Ferrier Jr.***, *Jennifer Imbrogno, Christina G. Rodriguez, Malgorzata Chwatko, Nathaniel A. Lynd*

4:30 Paper 36d: Dynamic Chemistry Leading to Full Property Recovery Associated with Crosslink Density in Reprocessed Polymer Networks and Network Composites: Network Synthesis by Step-Growth Reactions and by Nitroxide-Mediated Polymerization
— ***John M. Torkelson***, *Xi Chen, Kailong Jin, Lingqiao Li*

4:45 Paper 36e: Hybrid Chain-Growth/Step-Growth Mechanism Observed in Heterofunctional Thiol-Ene Polymerizations
— ***Dillon Love***, *Benjamin D. Fairbanks, Kang-Min Kim, Brady Worrell, Weixian Xi, J. Taylor Goodrich, Charles B. Musgrave, Mark Stoykovich, Christopher Bowman*

5:00 Paper 36f: High-Pressure Ethylene Polymerization with a Post-Metallocene Bis-Phenyl Phenoxy Catalyst
— ***Sean Ewart***, *Karjala Tom*

5:15 Paper 36g: A Simulation-Based Derivative-Free Optimization Framework Using the Kinetic Monte Carlo Method for Controlling Polymer Molecular Weight and Sequence Distribution Synthesized via Free-Radical Polymerization
— ***Hanyu Gao***, *Andreas Waechter, Ivan Konstantinov, Steven G. Arturo, Linda J. Broadbelt*

5:30 Paper 36h: Experimental and Macroscopic Mechanistic Modeling Studies of the Methyl Acrylate Self-Initiation Reaction
— *Hossein Riazi, Ahmad Arabi Shamsabadi, Michael Grady, Andrew M. Rappe,* ***Masoud Soroush***

5:45 Paper 36i: A Mathematical Model Based on Artificial Neural Network for Ethylene/Norbornene Copolymerization Catalyzed by 2-(tetramethylcyclopentadienyl)-4,6-Di-Tert-Butylphenoxytitanium Dichloride — ***Nikhil Prakash***

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(37) Quantitative Approaches to Disease Mechanisms and Therapies I
Sunday, Oct 29, 3:30 PM
MCC, 207A/B

Stacey D. Finley, Chair
Belinda S. Akpa, Co-Chair

Sponsored by:
Engineering Fundamentals in Life Science

3:30 Paper 37a: Towards the Optimal Design of a Minimal Set of Clinical Tests for the Identification and Characterization of Von Willebrand Disease
— *Beatrice Taverna, Alessandra Casonato, Fabrizio Bezzo,* ***Federico Galvanin***

3:48 Paper 37b: Experimental Verification of Endothelial Cell Aquaporin-1 Expression's Influence on Sub-Endothelial Intima Thickness and Relevance to Early Atherosclerosis
— *Roman Yakobov, Klaudio Mitri, Deyvi Tenemaza, Kung-Ming Jan,* ***David Rumschitzki***

4:06 Paper 37c: Mathematical Modeling and Data Analytics Using WBC Populations for the Prognosis and Diagnosis of Acute Coronary Syndrome
— ***Anwesha Chaudhury***, *John Higgins*

4:24 Paper 37d: Impact of Red Blood Cell Rigidity on the Vascular Wall Adhesion of Neutrophils: Implication in the Pathology of Sickle Cell Disease
— ***Mario Gutierrez***, *Margaret Fish, Omolola Eniola Adefeso*

4:42 Paper 37e: Model-Based Novel Strategy for Individualized Treatment of Sickle Cell Disease with Hydroxyurea
— ***Akancha Pandey***, *Robert Hannemann, Monica Khurana, Seethal Jacob, Terry Vik, Sangtae Kim, Doraiswami Ramkrishna*

5:00 Paper 37f: M2-Mediated Influenza Virus Budding and Scission: From Basic Principles to Control
— ***Jesper J. Madsen***, *John M. A. Grime, Gregory A. Voth*

5:18 Paper 37g: Transport of Molecular Motors on Networks of Cytoskeletal Filaments
— ***Paul J. Mlynarczyk***, *Steven M. Abel*

5:36 Paper 37h: Pathway Analysis of Combined In-Utero Exposure to Heavy Metals and Phthalates and Its Association with Child Psychomotor Development
— ***Dimosthenis Sarigiannis***, *Nafsika Papaioannou, Aikaterini Gabriel, Kinga Polanska, Evangelos Handakas, Spyros Karakitsios*

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(38) Reaction Engineering of Biomass and Hydrocarbons in Supercritical Water
Sunday, Oct 29, 3:30 PM
MCC, 102F

Michael T. Timko, Chair
Soumya Gudiyella, Co-Chair
Ki-Hyouk Choi, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

3:30 Paper 38a: Hydrothermal Upgrading of Algal Bio-Oil by Supercritical Water
— ***Akbar Saba***, *M. Toufiq Reza, Feng Cheng, Umakanta Jena, Catherine E. Brewer*

3:52 Paper 38b: Model Aldehyde Chemistry Using CeZrOx Catalyst for Hydrothermal Liquefaction Upgrading
*— **Alex Maag**, Geoffrey Tompsett, Alex D. Paulsen, Ted J. Amundsen, Paul E. Yelvington, Michael T. Timko*

4:14 Paper 38c: Hydrothermal Liquefaction of Wild-Harvested Cyanobacteria from a Hypereutrophic Lake in Wisconsin
*— **Megan Swoboda**, Yuanhui Zhang, Aersi Aierzhati, Wan-Ting Chen, Peng Zhang*

4:36 Paper 38d: Multiscale Modeling of Heavy Oil Upgrading in Near-Critical/Supercritical Water
*— **Ashwin Raghavan**, Ping He, Ahmed F. Ghoniem*

4:58 Paper 38e: Effects of Process Conditions on Metal Content in Biocrude from Hydrothermal Liquefaction of Microalgae
*— **Jimeng Jiang**, Phillip E. Savage*

5:20 Paper 38f: Bio-Crude Quality and Composition from Algal Solids Cultivated in Varying Media, Growth Stage, and Solids Loading
*— **Robert Hable**, Sirwan Alimoradi, Amanda C. Ruhmann, Andrew Doerflinger, Belinda S. M. Sturm, Susan M. Stagg-Williams*

5:42 Paper 38g: Thermal Chemistry of Alkylaromatics Reconsidered
*— **Lawrence Lai**, Soumya Gudiyella, Mengjie Liu, William H. Green*

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(39) Recent Advances in Molecular Simulation Methods I
Sunday, Oct 29, 3:30 PM
MCC, 200A

Erik E. Santiso, Chair
Cameron F. Abrams, Co-Chair
Harish Vashisth, Co-Chair

Sponsored by:
Computational Molecular Science and Engineering Forum

3:30 Paper 39a: Contact Freezing vs. Surface Freezing in Water
*— **Amir Haji-Akbari***

3:45 Paper 39b: Modeling the Homogeneous and Heterogeneous Nucleation of Crystals of Ionic Liquids in Different Environments
*— Yan Shen, Xiaoxia He, Erik E. Santiso, **Francisco R. Hung***

4:00 Paper 39c: Using Transition Path Sampling to Determine the Mechanism of the FCC-HCP Phase Transformation in Solid A
*— Bingxi Li, Artem Oganov, **Roland Faller***

4:15 Paper 39d: Using Metadynamics to Resolve and Characterize Complex Reactions at the Molecular Scale
*— **Christopher Fu**, Jim Pfaendtner*

4:30 Paper 39e: Improving Ab-Initio Molecular Dynamics Simulations of Water with Experimental Data
*— **Andrew White***

4:45 Paper 39f: Predicting Hydrogen-Deuterium Exchange Rates in Proteins Using Molecular Dynamics Simulations
*— **Harish Vashisth***

5:00 Paper 39g: Using Semidefinite Programming to Calculate Bounds on Stochastic Chemical Kinetic Systems
*— **Garrett R. Dowdy**, P. I. Barton*

5:15 Paper 39h Automated Discovery of Reaction Pathways for the Combustion of Alternative Fuel Candidates
*— **Ahmed E. Ismail***

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(40) Rechargeable / Secondary Battery Technologies for Energy Storage
Sunday, Oct 29, 3:30 PM
MCC, 200F

Burcu Gurkan, Co-Chair

Sponsored by:
Transport and Energy Processes

3:30 Paper 40a: Session Keynote: Ionic Liquid Electrolytes for Electrochemical Energy Storage
*— **Burcu Gurkan***

3:45 Paper 40b: A Novel Lithium Salt Additive for Improving Electrochemical Performance of High-Voltage $LiNi_{0.5}Mn_{1.5}O_4$ Cathode
*— **Juntian Fan**, Suojiang Zhang, Shimou Chen, Tao Dong*

4:00 Paper 40c: In-Situ Generation of Stable Interphases in Lithium-Oxygen Battery
*— **Snehashis Choudhury**, Lynden A. Archer*

4:15 Paper 40d: A Freestanding Calcium Hydroxide Interlayer as a Selective Separator for Rechargeable Alkaline Zn/MnO_2 Batteries
*— **Jinchao Huang**, Gautam G. Yadav, Joshua W. Gallaway, Michael Nyce, Xia Wei, Sanjoy Banerjee*

4:30 Paper 40e: Exploration of Key Descriptors of Solid Electrolyte Interphase Formation in Lithium-Ion Batteries Through Atomistic Simulations
*— **Mathew J. Boyer**, Gyeong S. Hwang*

4:45 Paper 40f: Regenerable Cu-Intercalated MnO_2-Layered Cathode for Highly Cyclable Energy-Dense Aqueous-Based Batteries
*— **Gautam G. Yadav**, Joshua Gallaway, Damon Turney, Jinchao Huang, Xia Wei, Michael Nyce, Sanjoy Banerjee*

5:00 Paper 40g: Investigation of Redox Active Oligomers for Nonaqueous Flow Batteries
*— **Jeffrey A. Kowalski**, Katharine V. Greco, Yu Cao, Jeffrey S. Moore, Fikile Brushett*

5:15 Paper 40h: An Analytical Model to Optimize the Cost-Effectiveness of Flow Batteries for the Electrical Grid
*— **Rose X. Ma**, Brian P. Setzler, Yushan Yan*

5:30 Paper 40i: Development of a Dynamic Model and Thermal Management Strategies for High-Temperature Sodium Sulfur Batteries
*— **Sai Pushpitha Vudata,** Debangsu Bhattacharyya, Richard Turton*

5:45 Paper 40j: Cycle Life Study and Failure Analysis of the Rechargeable Porous Zinc Electrode in Alkaline Electrolyte
*— **Michael D'Ambrose**, Sanjoy Banerjee, Robert Messinger, Gautam G. Yadav, Damon Turney, Joshua Gallaway, Michael Nyce*

6:00 Paper 40k: Degradation Modeling of Nickel-Rich Nickel-Cobalt-Manganese Oxide Cathode
*— **Jinseok Hong**, Changhoon Jung, Seung-Woo Seo, Kyoungmin Min, Hyo Sug Lee, Eunseog Cho*

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(41) Science and Engineering of Catalyst Preparation
Sunday, Oct 29, 3:30 PM
MCC, 103C

John R. Regalbuto, Chair
Praveen Bollini, Co-Chair
Homa Khosravian, Co-Chair
Xueyi Zhang, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

3:30 Paper 41a: Tailoring Zeolite ZSM-5 Crystal Morphology and Spatial Distribution of Acid Sites
*— **Wei Qin**, Matthew Patton, Jeffrey Rimer*

3:50 Paper 41b: Carbon Nanotube-Supported Catalysts Prepared by a Modified Photo-Fenton Process for Fischer-Tropsch Synthesis
*— **Haider Almkhelfe**, Xu Li, Keith Hohn, Placidus B. Amama*

4:10 Paper 41c: Synthesis Gas Conversion over Rh-Based Catalysts Promoted by Fe and Mn
*— **Yifei Liu**, Florian Göltl, Insoo Ro, Madelyn Ball, Isaias B. Aragão, Daniela Zanchet, George W. Huber, Manos Mavrikakis, James Dumesic*

4:30 Paper 41d: Tailored CeO_2-Supported Ni-Based Catalysts Prepared by Solution Combustion Synthesis for Hydrogen Generation from Hydrous Hydrazine
*— **Wooram Kang**, Arvind Varma*

4:50 Paper 41e: Synthesis of Rhodium Nanoclusters on Graphene/Cu(111) from Organometallic Precursors: A Combined DFT and STM Study
*— **Elizabeth Montiel-Macias**, Perla Balbuena, Homa Khosravian*

5:10 Paper 41f: Adsorption of Transition Metal Precursors on Reducible Metal Oxide Supports: Toward Rational Synthesis of Single-Site Catalysts
*— **Ahana Mukhopadhyay**, Robert M. Rioux*

5:30 Paper 41g: Nanoparticle Synthesis via Electrostatic Adsorption Using Incipient Wetness Impregnation
*— **Sonia Eskandari**, John R. Regalbuto*

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(42) Self- and Directed Assembly at the Nanoscale
Sunday, Oct 29, 3:30 PM
MCC, 213A/B

Anju Gupta, Chair
Javen Weston, Co-Chair
Megan A. Creighton, Co-Chair

Sponsored by:
Nanoscale Science and Engineering Forum

3:30 Paper 42a: Topographic Pattern-Directed Ordering and Dewetting of Phase-Segregated Domains in Polymer-Blend Thin Films
*— **Rabibrata Mukherjee**, Nandini Bhandaru*

3:47 Paper 42b: Designing Iron Oxide–Metal-Organic Framework Superstructures by Ligand-Mediated Self-Assembly
*— **Fen Qiu**, Yanfang Zhang, Guo Li, Jeffrey Neaton, Jeffrey Urban*

4:04 Paper 42c: Structural Analysis and Simulation of Colloidal Clathrate Crystals Self-Assembled from DNA-Functionalized Gold Nanoparticles
*— **Sangmin Lee**, Michael Engel, Matthew Spellings, Sharon C. Glotzer*

4:21 Paper 42d: 3D Carbon Nanomaterial/Metal Nanowire Hybrid Composite Electrodes via Electrostatic Self-Assembly for Energy Storage and Conversion
*— **Enoch Nagelli**, COL F. John Burpo, MAJ Stephen Winter*

4:38 Paper 42e: Shear-Induced Structural Transitions and Gelation in Ultra-Low Interfacial Tension Microemulsions
*— **Javen Weston**, Kathleen Weigandt*

4:55 Paper 42f: Oriented Attachment of Ag Nanoplates: A Molecular Dynamics Study
*— **Tonnam Balankura**, Kristen Fichthorn*

5:12 Paper 42g: Molecular Insights in Self-Assembly of Di-FMOC-L-Lysine in Organic Solvent/Water Mixtures
*— Md. Masrul Huda, Meysam Hashemnejad, Santanu Kundu, **Neeraj Rai***

5:29 Paper 42h: Redox-Directed Self-Assembly of 2D Semiconductor Nanoantenna Heterostructures with Enhanced Optoelectronic Damping and Nonlinear Activity
*— **D. Keith Roper**, Gregory T. Forcherio, Jeremy Dunklin, Mourad Benamara, Luigi Bonacina*

5:46 Paper 42i: Fine-Tuning the Release Rate of Paclitaxel-Bearing Supramolecular Filament Hydrogels
*— **Rami Chakroun**, Feihu Wang, Ran Lin, Yin Wang, Hao Su, Honggang Cui*

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(43) Solids Handling and Processing in the Chemical Industry: What They Don't Teach You at School
Sunday, Oct 29, 3:30 PM
MCC, 200J

Shrikant Dhodapkar, Chair
George Klinzing, Co-Chair

Sponsored by:
Solids Flow, Handling and Processing

3:30 Paper 43a: Practical Approaches for Troubleshooting Solids Processing Systems *— **Shrikant Dhodapkar, George Klinzing, Ray Cocco, Patrick T. Spicer, Manuk Colakyan***

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(44) Supply Chain Logistics and Optimization
Sunday, Oct 29, 3:30 PM
MCC, 103F

Chrysanthos E. Gounaris, Chair
Fengqi You, Co-Chair

Sponsored by:
Computers in Operations and Information Processing

3:30 Paper 44a: Supply Chain Logistics for Personalized Medicines
*— **Xiaonan Wang,** Nilay Shah*

3:51 Paper 44b: A Dynamic Game Theoretic Framework for Strategic Production Planning
*— **Philip Tominac**, Vladimir Mahalec*

4:12 Paper 44c: Optimal Supply Chain Network Design for the Upstream Sector of the Oil and Gas Industry
*— **Agustin F. Montagna, Diego C. Cafaro***

4:33 Paper 44d: Mixed-Integer Models for Simultaneous Optimization of Safety Stock and Inventory Policies in Supply Chain Planning
*— **Braulio Brunaud**, José Miguel Laínez-Aguirre, Jose M. Pinto, Ignacio E. Grossmann*

4:54 Paper 44e: Modeling and Optimization of Multi-Product Supply Chains
*— **Victor M. Zavala,** Mariano Martin, Apoorva Sampat, Edgar Martin*

5:15 Paper 44f: A Branch-Price-and-Cut Approach for Robust Optimization in Vehicle Routing
*— **Akang Wang**, Chrysanthos E. Gounaris*

5:36 Paper 44g: Allocation and Transportation Optimization of Products to Contracts Under Multiple, up to Second-Order, Statistics Conditions on a Variable List of Product Characteristics
*— **Chris Domnisoru***

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(45) Sustainable Electricity: Generation and Storage
Sunday, Oct 29, 3:30 PM
MCC, 101C

Sheila Samsatli, Chair
Vilas G. Pol, Co-Chair

Sponsored by: Sustainable Energy

3:30 Paper 45a: Power Capacity Expansion Planning Considering Endogenous Technology Cost Learning
*— **Clara F. Heuberger**, Edward S. Rubin, Iain Staffell, Nilay Shah, Niall Mac Dowell*

3:51 Paper 45b: Data-Driven Battery Sizing and Market Participation
*— **Alexander W. Dowling**, Farshud Sorourifar, Jose A. Renteria, Victor M. Zavala*

4:12 Paper 45c: Techno-Economic and Environmental Optimization of Wind Farm with Energy Storage Systems
*— Jiajun Cen, **Xiaonan Wang***

4:33 Paper 45d: Hybrid Renewable Energy System Evaluation for Industry Applications
*— **Eduardo Vyhmeister**, Lorenzo Reyes-Bozo, Carlos Funez-Guerra, Héctor Valdés-González, Cristina Aleixendri-Muñoz*

4:54 Paper 45e: Sustainable Planning of Urban Energy-Water-Food Nexus Through Decision-Making Tools
*— Niclas Bieber, Jen Ho Ker, **Xiaonan Wang**, Nilay Shah*

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(46) Workshop: Effective Teaching for New or Prospective Faculty
Sunday, Oct 29, 3:30 PM
MCC, 205C

Lisa G. Bullard, Co-Chair
Donald P. Visco Jr., Co-Chair
David L. Silverstein, Co-Chair

Sponsored by: Education

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(47) Workshop: Inexpensive Microcontrollers in Any ChE Course
Sunday, Oct 29, 3:30 PM
MCC, 205D

Daniel D. Burkey, Co-Chair
Anthony Edward Butterfield, Co-Chair
Daniel Anastasio, Co-Chair
Kyle Branch, Co-Chair

Sponsored by:
Undergraduate Education

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(48) Advanced Fuel Cell, Hydrogen Generation & Storage Technologies
Monday, Oct 30, 8:00 AM
MCC, 200F

Sponsored by:
Transport and Energy Processes

8:00 Paper 48a: Session Keynote: Beneficial Uses of Stranded Assets — Emerging Opportunities
*— **Pinakin Patel**, Ludwig Lipp*

8:22 Paper 48b: Session Keynote: Low-Carbon Power Generation with Methane-Fueled SOFCs
*— **Yoshio Matsuzaki**, Yasuharu Kawabata, Yuya Tachikawa, Martin Keller, Junichiro Otomo, Shunsuke Taniguchi, Kazunari Sasaki*

8:44 Paper 48c: Performance Modeling of Materials-Based Hydrogen Storage Systems for Automotive Applications
*— **Kriston Brooks**, David A. Tamburello, Sam Sprik, Matthew J. Thornton*

9:06 Paper 48d: Metal Oxide–Based Two-Step Solar-Driven Methane Reforming and H_2O/CO_2 Splitting Thermochemical Cycle
*— **Rahul Bhosale**, Parag N. Sutar, Gorakshnath Takalkar*

9:28 Paper 48e: Immobilized Ferrite Nanoparticles for H_2 Generation via Low-Temperature Thermochemical Water-Splitting Process
*— **Vinod S. Amar**, Rajesh V. Shende, Jan A. Puszynski*

9:50 Paper 48f: Application of Liquid Organic Hydrogen Carrier in Mobility
*— **Wolfgang Arlt**, Daniel Teichmann, Jonas Obermeier*

10:12 Paper 48g: Super-Saturation of Nitrogen and Hydrogen in Transition Metals and Metal Hydrides/Nitrides
*— **Peter C. Psarras**, Jennifer Wilcox*

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(49) Advanced Oxidation Processes I
Monday, Oct 30, 8:00 AM
MCC, 102F

Robert W. Peters, Chair
Mohammed Mostafa, Co-Chair
Tapas K. Das, Co-Chair
Selma Mededovic Thagard, Co-Chair

Sponsored by: Water

8:00 Paper 49a: Photodegradation of Pharmaceuticals in Partially Nitritated Wastewater
*— **Priya I. Hora**, Paige J. Novak, William A. Arnold*

8:25 Paper 49b: Oxidation of High-Molecular-Weight Dye Using Ozone Isotopomers
*— Kishora K. Panda, **Alexander P. Mathews***

8:50 Paper 49c: Removal of Algal Matter by Coagulation Both in Presence and Absence of Pre-Oxidation
*— **Ziming Zhao,** Madhumita B. Ray, Hassan Gomaa*

9:15 Paper 49d: Ozone Microbubble and Its Use in Arsenic Removal from Waste Water
*— **Subrata Kumar Majumder***

9:40 Paper 49e: An Efficient Degradation of Perchloroethylene by Nano Zero Valent Iron (nZVI) and nZVI-Activated Sodium Percarbonate with and Without Addition of Ethylenediaminetetraacetic Acid Disodium Salt Dehydrate
*— **Muhammad Danish**, Shuguang Lu, Usman Farooq, Sadiq Hussain, Ayyaz Ahmad, Muhammad Naqvi, Mujtaba Ashraf, Abdul Sattar Qureshi, Xiaori Fu*

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(50) Advances in Membrane Technologies for Food and Bioprocessing
Monday, Oct 30, 8:00 AM
MCC, 206A/B

Gaohong He, Chair
Chuang Xue, Co-Chair
Xiaobin Jiang, Co-Chair

Sponsored by: Food

8:00 Paper 50a: Functional Graphene Oxide Coating with Speek Coaxial Electrospun Fibers for Proton Exchange Membranes
*— **Xuemei Wu**, Fujun Cui, Xiaoming Yan, Yao Wu, Wanting Chen, Gaohong He*

8:18 Paper 50b: Performance of a Submerged Anaerobic Membrane Bioreactor (AnMBR) at Long HRT and High Solid Concentration: Focusing on Membrane Fouling and Effluent Quality
*— Yifru Waktole Berkessa, Binghua Yan, **Ming Tan**, Yang Zhang*

8:36 Paper 50c: Mixed-Matrix Membranes for Butanol Recovery Based on Zeolites as Macro-Crosslinkers
— ***Peiyong Qin***, *Song Hu Sr.*

8:54 Paper 50d: What Causes Fuel Cell Membranes to Dry Out?
— ***Jay Benziger***, *Ioannis G. Kevrekidis, Yannick DeDecker*

9:12 Paper 50e: Polyarylester Nanofiltration Membranes with Solvent Resistance
— ***Yan Fu***, *Ayang Zhou, Jinli Zhang, Wei Li*

9:30 Paper 50f: Bipolar Membrane Electrodialysis for Cleaner Production of Amino/Organic Acids
— ***Yaoming Wang***, *Xiaoli Wang, Chenxiao Jiang,* ***Tongwen Xu***

9:48 Paper 50g: Cross-Linked Mixed-Matrix Membranes for Organic Solvent Nanofiltration (OSN) Consisting of P84 Polyimide and Carboxyl-Functionalized Multi-Walled Carbon Nanotubes
— ***Mohammad Hossein Davood Abadi Farahani***, *Dan Hua, Tai-Shung Chung*

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(51) Area Plenary: Emerging Areas in Polymer Science and Engineering I — Area 8A (Invited Talks)
Monday, Oct 30, 8:00 AM
MCC, 211B

Ying Diao, Chair
Santanu Kundu, Co-Chair

Sponsored by: Polymers

8:00 Paper 51a: Mechanical Properties of Organic Semiconductors for Mechanically Stable and Intrinsically Stretchable Solar Cells
— ***Darren Lipomi***

8:35 Paper 51b: Digital Light Synthesis to Drive Additive Manufacturing
— ***Joseph M. DeSimone***

9:10 Paper 51c: Symbiotic Pairing of Near-UV Solar Cells with Electrochromic Windows for Visible Light and Heat Management in Architectural Applications
— ***Y. L. Lynn Loo***

9:45 Paper 51d: Taking Measure of Modern Polymer Synthesis
— ***Kathryn L. Beers***

(52) Atomically Dispersed Supported Metal Catalysts I
Monday, Oct 30, 8:00 AM
MCC, L100F

Lars C. Grabow, Chair
Maria Flytzani-Stephanopoulos, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

8:00 Paper 52a: Escaping Linear Scaling Relations: Catalysis Beyond Constraints on Single-Atom Alloys
— *Matthew Darby, Angelos Michaelides,* ***Michail Stamatakis***

8:40 Paper 52b: Mechanistic Studies of Selective Hydrogenation Reactions with Palladium Gold Alloy Catalysts
— ***Jilei Liu***, *Junjun Shan, Antonios Trimpalis, Sufeng Cao, Maria Flytzani-Stephanopoulos*

9:00 Paper 52c: Thermally Stable Single-Atom Pt/m-Al_2O_3 for CO Oxidation and the Selective Hydrogenation of 1,3-Butadiene
— ***Ning Yan***

9:20 Paper 52d: Interactions of Water and Chiral Properties of a Single-Site Pt "29" Cu_xO/Cu(111) Catalyst
— ***Kyle Groden***, *Alyssa Hensley, Alex C. Schilling, Andrew Therrien, Renqin Zhang, E. Charles H. Sykes, Jean-Sabin McEwen*

9:40 Paper 52e: Spectroscopic Signatures and Reactivity of CO Adsorbed to Atomically Dispersed Pt Atoms, Pt Oxide Clusters, and Metallic Pt Clusters on Anatase TiO_2
— ***Leo DeRita***, *Sheng Dai, Kimberly Lopez-Zepeda, Nicholas Pham, Phillip Christopher*

10:00 Paper 52f: Reversible Transformation from Pt Single Atoms to Sub-Nanometer Particles for Low-Temperature CO Oxidation
— ***Xavier Isidro Pereira Hernández***, *Andrew T. DeLaRiva, Haifeng Xiong, Eric J. Peterson, Deepak Kunwar, Berlin Sudduth, Yong Wang, Abhaya K. Datye*

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(53) Big Data and Sustainability
Monday, Oct 30, 8:00 AM
MCC, 101D

Nastassja Lewinski, Chair
Cory Jensen, Co-Chair
William M. Barrett, Co-Chair

Sponsored by: General

8:00 Paper 53a: Theory-Guided Data Science: A New Paradigm for Scientific Discovery in the Era of Big Data
— ***Anuj Karpatne***

8:26 Paper 53b: DeepMetabolism: A Deep Learning System to Predict Phenotype from Genome Sequencing
— ***Weihua Guo***, *You Xu, Xueyang Feng*

8:52 Paper 53c: Comparison of Ozone Analyses Between Camx and DENFIS for Selected Monitoring Sites in an Ozone Nonattainment Area
— ***Xiaonan Xu***, *Jian Zhang, Qiang Xu, Thomas Ho*

9:18 Paper 53d: Design of an Integrated Renewable and Conventional Resources-Based Energy Supply System Coupled with CCS (IRCEC) System Using Multi-Objective Optimization
— ***Minsoo Kim***, *Sunghoon Kim, Jiyong Kim*

9:44 Paper 53e: Data Analysis of Global Waste Plastic Mismanagement to Identify Critical Locations for Implementing Sustainable Abatement Strategies
— ***Chandni Joshi***, *Jeffrey R. Seay*

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(54) Biofuels Production: Design, Simulation, and Economic Analysis
Monday, Oct 30, 8:00 AM
MCC, 101B

Ramalingam Subramaniam, Chair
Mark Mba Wright, Co-Chair
Ana I. Torres, Co-Chair

Sponsored by:
Sustainable Biorefineries

8:00 Paper 54a: Techno-Economic Analysis (TEA) of Auto-Thermal Pyrolysis of Lignocellulosic Biomass to Transportation Fuels — ***Wenqin Li***

8:21 Paper 54b: Process Synthesis and Economical Evaluation of Torrefied Wood Pellet Production Processes
— ***Huimin Yun***, *Roland Clift, Xiaotao Bi*

8:42 Paper 54c: Implementation of Six Sigma in a Methane Generation Process — ***Manohar Manchenahalli***, *Joseph D. Smith, Haider Al-Rubaye, Shruti Karambelkar*

9:03 Paper 54d: Performance of Fed-Batch Relative to Batch Processes in Unsteady-State Fermentation and In-Situ Gas Stripping Simulations Under Different Conditions
— ***Kwabena Darkwah***, *Jeffrey Seay, Barbara L. Knutson*

9:24 Paper 54e: Technoeconomic Assessment of Biofuel and Biochemical Production Using New Pretreatment Processes for Lignocellulosic Biomass and Lignin Valorization
— ***Peyman Fasahati***, *Christopher M. Saffron*

9:45 Paper 54f: Technoeconomic and Strategic Insights on Cellulosic Biofuel Production with Ionic Liquid Pretreatment
— ***N.V.S.N. Murthy Konda***, *Seema Singh, Jian Sun, Binod Neupane, Blake A. Simmons, Corinne D. Scown*

10:06 Paper 54g: Process Simulation of Integrated Biomass Torrefaction and Pelleting Plant — ***Maryam Manouchehrinejad***, *Sudhagar Mani*

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(55) Biomaterials: Faculty Candidates
Monday, Oct 30, 8:00 AM
MCC, 211C

Angela K. Pannier, Chair
Steven R. Caliari, Co-Chair
Ryan Koppes, Co-Chair
Lorraine Leon, Co-Chair

Sponsored by: Biomaterials

8:00 Paper 55a: Rational Design of Polyelectrolyte Complexes for Nucleic Acid Delivery
— ***Jeffrey Vieregg***, *Matthew V. Tirrell*

8:18 Paper 55b: Microfabricated Immune-Isolating Devices for Long-Term Cell-Based Therapies
— ***Suman Bose***, *Robert Langer, Daniel Anderson*

8:36 Paper 55c: Globular Protein Vesicles: Engineering Vesicle Size and Membrane Structure Through a Tunable Molecular Packing Parameter
— ***Yeongseon Jang,*** *Julie A. Champion*

8:54 Paper 55d: Biomaterial Scaffolds for Scalable Differentiation and Transplantation of hPSC-Derived Cells for Cell Replacement Therapy in the Central Nervous System
— ***Maroof M. Adil***, *David V. Schaffer*

9:12 Paper 55e: Functional Reconstitution and Characterization of Artificial Proton Channels in Artificial Membranes
— ***Yuexiao Shen***, *Istvan Kocsis, Mihai Barboiu, Manish Kumar*

9:30 Paper 55f: Electrochemical Activation for DNA Attachment to Surfaces
— ***Ariel Furst***, *Matthew Francis*

9:48 Paper 55g: Organizing Biochemical Reactions with Protein Droplets — ***Huaiying Zhang***

10:06 Panel Discussion

(56) Bionanotechnology for Gene and Drug Delivery II
Monday, Oct 30, 8:00 AM
MCC, 212A/B

Joo Youp Lee, Chair
Elizabeth Nance, Co-Chair
Yoonjee Park, Co-Chair
Aaron C. Anselmo, Co-Chair

Sponsored by: Bionanotechnology

8:00 Paper 56a: Carbon Nanotube-Assisted Delivery of Genetic Material into Mature Plants — ***Gozde Sultan Demirer***, *Markita Landry*

8:18 Paper 56b: On-Demand Delivery and Monitoring of Drug
— ***Yoonjee Park***, *Zhe Zhang, Madison Taylor*

8:36 Paper 56c: Drug Release from Nanoparticles: Modulating Hydrophobic Prodrug Degradation Rates with Lipid Excipients
— ***Brian K. Wilson***, *Robert K. Prud'homme*

8:54 Paper 56d: Peptide-Modified Liposomes for Treatment of Multiple Myeloma via Selective Targeting of CD138 and Dual Targeting of CD138 and VLA-4
— ***David Omstead***, *Matt Lecinski, Tanyel Kiziltepe, Basar Bilgicer*

9:12 Paper 56e: Modulating *Pseudomonas aeruginosa* Bacterial Communication with Nanoformulated Signaling Agents
— ***Kurt D. Ristroph***, *Hoang Lu, Elizabeth Pearson, Gregg Duncan, Laura Ensign, Jung Soo Suk, Justin Hanes, Robert Prud'homme*

9:30 Paper 56f: Nanoparticle-Supported Lipid Bilayers for Drug Delivery
— ***Alexander L. Kelly***, *Robert D. Arnold, Allan E. David*

9:48 Paper 56g: Fusion of Outer Membrane Vesicles: Surface-Display of Different Epitopes on a Single Vesicle
— ***Yehou Gnopo,*** *Aditya Mirsa, Yeo Eun Kim, Matthew P. DeLisa, Susan Daniel, David Putnam*

10:06 Paper 56h: Precision Nanomedicines to Deliver Kinase Inhibitors to the Tumor Microenvironment
— ***Daniel Heller***, *Yosi Shamay*

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(57) Carbon Dioxide Capture from Power Generation
Monday, Oct 30, 8:00 AM
MCC, 200C

David Hopkinson, Chair
Zachary Smith, Co-Chair

Sponsored by:
Advances in Fossil Energy R&D

8:00 Paper 57a: Analysis of Post-Combustion Inertial CO_2 Extraction System — *Adam H. Berger, Yuqi Wang, Anthony Castrogiovanni, Robert Kielb, Vladimir Balepin,* ***Abhoyjit S. Bhown***

8:19 Paper 57b: Highly Efficient Warm Gas Carbon Capture System for IGCC Power Plants
— ***Ambalavanan Jayaraman***, *Gokhan Alptekin, Michael Bonnema*

8:38 Paper 57c: The Development of a Data Mining–Molecular Modeling Approach to Screen Physical Solvents for Gas Separation
— *David Hopkinson,* ***Wei Shi***

8:57 Paper 57d: Influence of Solvent Molecular Structure on Energy Consumption of Post-Combustion CO_2 Capture Processes
— *Kevin G. Joback, J. R. Heberle,* ***Abhoyjit S. Bhown***

9:16 Paper 57e: Process Modeling and Optimization of a Novel Membrane-Assisted Chilled Ammonia Process for CO_2 Capture
— ***Ryan Hughes***, *Goutham Kotamreddy, Debangsu Bhattacharyya, Michael Matuszewski*

9:35 Paper 57f: Design and Operations Optimization of Membrane Separation for Flexible Carbon Capture from Natural Gas Combined-Cycle Systems
— ***Mengyao Yuan***, *Holger Teichgräber, Jennifer Wilcox, Adam Brandt*

9:54 Paper 57g: Technical and Economic Feasibility Study of Membranes for Carbon Capture from Low-CO_2-Concentration Sources
— ***Yang Han***, *W. S. Winston Ho*

10:13 Paper 57h: Doping Polybenzimidazole (PBI) with Phosphoric Acid to Enhance Membrane H_2/CO_2 Separation Properties
— ***Lingxiang Zhu***, *Mark T. Swihart, Haiqing Lin*

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(58) Catalytic Processing of Fossil and Biorenewable Feedstocks I: Lignin and Bio-Oil Chemistry
Monday, Oct 30, 8:00 AM
MCC, L100C

Jeremy S. Luterbacher, Chair
Julia A. Valla, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

8:00 Paper 58a: Hydrodeoxygenation of Anisole as Bio-Oil Model Compound over Supported Non-Sulphided CoMo Catalysts: Effect of Co/Mo Ratio and Support
— ***Chanakya Ranga***, *Rune Lødeng, Vaios I. Alexiadis, Joris W. Thybaut*

8:20 Paper 58b: Sulfur-Tolerant Molybdenum Carbide Catalysts Enabling Low-Temperature Stabilization of Fast-Pyrolysis Bio-Oil
— *Zhenglong Li,* ***Jae-Soon Choi***, *Huamin Wang, Andrew W. Lepore, R. Maggie Connatser, Samuel A. Lewis Sr., Harry M. Meyer III, Alan H. Zacher*

8:40 Paper 58c: Controlling Selectivity of Bio-Oil Model Compound Upgrading with Metal Promoters on Molybdenum Carbide — ***Sarah W. Paleg,*** *Levi T. Thompson*

9:00 Paper 58d: Reductive Conversion of Lignin with Copper-Doped Catalysts
— ***Marcus Foston***

9:20 Paper 58e: Hierarchical Nickel-Incorporated USY Zeolites for Hydrodeoxygenation of Lignin-Derived Pyrolysis Oil Model Compounds
— ***David P. Gamliel***, *Julia A. Valla*

9:40 Paper 58f: *Operando* Solid-State NMR Study of Hydrogenolysis of Lignin Ether Linkages
— ***Long Qi***, *Ali Chamas, David W. Hoyt, Eric D. Walter, Nancy M. Washton, Susannah L. Scott*

10:00 Paper 58g: In-Situ Spectroscopy of Lignin Disassembly
— ***Marcus Foston***, *Susannah L. Scott, Long Qi, Sai V. Pingali, David Hoyt, Nancy M. Washton*

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(59) Characterization of Composites
Monday, Oct 30, 8:00 AM
MCC, 211D

Lalitha V. N. R. Ganapatibhotla, Chair
Zhen Liu, Co-Chair
Liwen Mu, Co-Chair

Sponsored by: Composites

8:00 Paper 59a: Electron Energy Loss Spectroscopy for Optoelectronics and Thermal Dynamics at Nanocomposite Interfaces
— ***D. Keith Roper***, *Jeremy Dunklin, Gregory T. Forcherio, Keith Berry, Carter Bodinger, Tyler Howard*

8:18 Paper 59b: On the Rice Husk Ash Admixing with Cement: Preparation, Characterization and Analysis
— ***Nikhil Prakash***

8:36 Paper 59c: Tunable Magnetoresistance of Conductive Polymer Nanocomposites
— ***Jiang Guo***, *Alexandra Galaska, Suying Wei, Brian J. Edwards, Bamin Khomami, Zhanhu Guo*

8:54 Paper 59d: Polydopamine-Stabilized Fluorescent Nanozinc Oxide–Reinforced Epoxy Nanocomposites Towards UV Shielding
— ***Chaobo Liang***, *Ping Song, Hongbo Gu, Junwei Gu*

9:12 Paper 59e: Comparing the Toughening Effects of Modified Graphene Oxide and Core-Shell Rubber on Polyester Resins and Glass Fiber-Reinforced Polyester Composites
— ***Kunwei Liu***, *Siyao He, Yuqiang Qian, Qi An, Andreas Stein, Christopher W. Macosko*

9:30 Paper 59f: Preparation and Characterizations of Barium Ferrite/Epoxy Nanocomposites
— ***Hongyuan Zhang***, *Hongbo Gu*

9:48 Paper 59g: Effect of Compatibilizer on Strength and Toughness of Glass Fiber Mat–Reinforced Polypropylene Composites
— ***Chunyin Shen***, *Yadong Wu, Haiqing Wan, Junyan Wang, Gance Dai*

10:06 Paper 59h: A Facile Approach to Fabrication and Characterization of an Eco-Friendly Zein-Laponite Nanocomposite with Improved Mechanical, Thermal, Barrier and Surface Property — ***Tahrima B. Rouf***

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(60) Characterization of Engineered Particles and Nanostructured Particulate Systems
Monday, Oct 30, 8:00 AM
MCC, 200H

M. Silvina Tomassone, Chair
Mohammad Azad, Co-Chair

Sponsored by:
Particle Production and Characterization

8:00 Paper 60a: Novel Computational Strategy for Particle Charge Determination
— ***Xikai Jiang***, *Jiyuan Li, Olle G. Heinonen, Juan J. de Pablo*

8:20 Paper 60b: Novel Applications of Light Scattering Techniques for On-Line Characterization of Nano-Particles
— ***Alon Vaisman***

8:40 Paper 60c: Core-Shell Nanostructured Anodes for Lithium-Ion Batteries
— ***Kurt B. Smith***, *M. Silvina Tomassone*

9:00 Paper 60d: Connecting the In-Operando Reduction Kinetics of Porous Nickel Oxide and Copper Oxide in Dilute H_2 from the Molecular to Micron Scales for Clean Energy Generation — ***Greeshma Gadikota***

9:20 Paper 60e: Non-Contact AFM Measurement of the Hamaker Constants for the Improvement of Trace Explosive Detection
— ***Sean G. Fronczak***, *Chris Browne, Elizabeth Krenek, D. S. Corti, Stephen P. Beaudoin*

9:40 Paper 60f: High-Resolution Characterization of Colloid Size Distributions by Field Flow Fractionation
*— **Tianying Jiang**, Erick Soto-Cantu, Charlie Chan*

10:00 Paper 60g: Monitoring Magnetic Nanoparticle Synthesis Progress Using a Benchtop Magnetic Particle Relaxometer
*— **Rohan Dhavalikar**, Justina Chan, Shehaab Savliwala, Mythreyi Unni, Nicolas Garraud, David P. Arnold, Carlos Rinaldi*

10:20 Paper 60h: Models for Powder Handling and Dosing in Air
*— **Reza Baserinia**, Csaba Sinka*

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(61) Division Plenary: CAST (Invited Talks)
Monday, Oct 30, 8:00 AM
MCC, 103C

Prodromos Daoutidis, Chair
Efstratios N. Pistikopoulos, Co-Chair

Sponsored by:
Computing Systems and Technology Division

8:00 Paper 61a: Overview of CAST Activities and Programming
*— **Efstratios N. Pistikopoulos**, **Prodromos Daoutidis***

8:25 Paper 61b: Process Synthesis Using Grid Superstructure
*— **Jianping Li**, Salih E. Demirel, M. M. Faruque Hasan*

8:50 Paper 61c: Stability and Performance of Economic Model Predictive Control with Discrete Actuators
*— **Michael Risbeck**, James B. Rawlings*

9:15 Paper 61d: Global Optimization Algorithm for Capacitated Multi-Facility Continuous Location-Allocation Problems
*— **Cristiana L. Lara**, Ignacio Grossmann*

9:40 Paper 61e: Nonlinear System Identification: Finding Normal Forms by Iteratively Uncovering Informed Geometries
*— **David Sroczynski**, Or Yair, Ronen Talmon, Ioannis G. Kevrekidis*

10:05 Paper 61f: Model-Predictive Safety System for Predictive Detection of Operation Hazards: Off-Line Calculation of Most Aggressive Control Actions and Worst-Case Uncertainties
*— **Masoud Soroush**, Jeffrey E. Arbogast, Warren D. Seider*

(62) Division Plenary: Chemical Engineering Principles for Nanotechnology (Invited Talks)
Monday, Oct 30, 8:00 AM
MCC, 213A/B

Geoffrey D. Bothun, Chair
Reginald E. Rogers Jr., Co-Chair

Sponsored by:
Nanoscale Science and Engineering Forum

8:00 Welcoming Remarks

8:05 Paper 62a: NSEF Forum Plenary: Mechanisms, Design and Fabrication of Non-Viral Gene Delivery Systems
*— **Daniel W. Pack.***

9:05 Intermission

9:15 Paper 62b: NSEF Young Investigator Award — Disorder, Nonequilibrium Transport, and the Critical Role of Size Dispersity in Colloidal Semiconductor Nanomaterials
*— **William A. Tisdale***

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(63) Division Plenary: Gerhold and Kunesh Awards on Separations (Invited Talks)
Monday, Oct 30, 8:00 AM
MCC, 101F

Mark M. Davis, Chair
Scott M. Husson, Co-Chair

Sponsored by: Separations Division

8:00 Paper 63a: Novel Membranes, Membrane Processes and Membrane Devices *— **Kamalesh K. Sirkar***

8:30 Paper 63b: Ion Sorption, Diffusion and Transport in Charged Polymer Membranes
*— **Benny D. Freeman***

9:00 Paper 63c: Bioinspired to Multifunctional Nanostructured Membranes
*— **Dibakar Bhattacharyya,** Hongyi Wan, Anthony Saad, Andrew Colburn, Ashish Aher, Rupam Sarma*

9:30 Paper 63d: FRI/John G. Kunesh Award Lecture — In Search of New Paradigms for Crystal Engineering: Old Tricks, Novel Discoveries, and Future Challenges *— **Jeffrey D. Rimer***

10:00 Paper 63e: Clarence G. Gerhold Award Lecture — Flexibility-Based Separations: A New Paradigm for Membranes *— **Andrew Zydney***

(64) Division Plenary: Imaging of Heavy Hydrocarbon Molecule Structures
Monday, Oct 30, 8:00 AM
MCC, 200A

Doug Kushnerick, Chair
Saadet Ulas Acikgoz, Co-Chair

Sponsored by:
Fuels and Petrochemicals Division

8:00 Introductory Remarks

8:05 Paper 64b: The Revolution of Atomic-Force Microscopy for Organics *— **Bruno Schuler***

8:25 Paper 64c: Pure Component Control Experiments
*— **Yunlong Zhang***

8:40 Paper 64d: Molecular Structure of Heavy Oil Revealed (1)
*— **Michael Moir***

8:55 Paper 64e: Molecular Structure of Heavy Oil Revealed (2)
*— **Frans Van den Berg***

9:10 Paper 64f: Molecular Structure of Heavy Oil Revealed (3)
*— **Bruno Schuler***

9:25 Paper 64g: Molecular Structure of Heavy Oil Revealed (4)
*— **Michael R. Harper***

9:40 Paper 64h: State of the Art in Characterizing Complex Hydrocarbon Mixtures, and What to Do with It
*— **Michael T. Klein***

9:58 Paper 64i: Perspectives on Catalyst Design for Complex Feedstocks
*— **Matthew Neurock***

10:16 Paper 64j: TBD TBD
*— **Paul J. Dauenhauer***

10:34 Panel Discussion, Q&A

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(65) Dynamics and Modeling of Particulate Systems I
Monday, Oct 30, 8:00 AM
MCC, 200J

Stefan Radl, Chair
Timothy M. Healy, Co-Chair

Sponsored by:
Solids Flow, Handling and Processing

8:00 Paper 65a: Extraction of Parameters for a Square-Force Cohesion Model from Defluidization Experiments
*— **Peiyuan Liu**, Casey Q. LaMarche, Kevin M. Kellogg, Christine M. Hrenya*

8:19 Paper 65b: Quantitative Simulation of Tablet Compression and Hardness Test Processes Using Discrete Element Method
*— **Yijie Gao***

8:38 Paper 65c: Simulating Convex Polyhedral Particles Utilizing the Discrete Element Method on GPU
*— **Eva Siegmann**, Johannes G. Khinast, Gundolf Haase*

8:57 Paper 65d: DEM Simulation Studies on the Effect of Particle Size and Morphology on Mixing and Fluid Content Uniformity in a Double-Cone Impregnator
*— **Yangyang Shen**, William G. Borghard, M. Silvina Tomassone*

9:15 Paper 65e: CFD-DEM Simulations and Uncertainty Quantification (UQ) of Horizontal Jets in Gas-Solid Fluidized Bed
*— **Peiyuan Liu**, William Fullmer, Steven R. Dahl, Christine M. Hrenya*

9:34 Paper 65f: Particle-Fluid Dynamic Code Validation with Hydrodynamic Experiments
*— Matthew A. Hamilton, **Zachary Reinking**, Kevin Whitty, JoAnn S. Lighty*

9:53 Paper 65g: Proppant Transport Efficiency Simulation in a Wellbore-Fracture System
*— **Jianxin Lu**, Andrey Filippov*

10:12 Paper 65h: Two-Compartment Modeling and Simulation Study of a Top-Sprayed Fluidized-Bed Granulator
*— **Gurmeet Kaur**, Mehakpreet Singh, Themis Matsoukas, Jitendra Kumar, Thomas De Beer, Ingmar Nopens*

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(66) Electrocatalysis and Photoelectrocatalysis I: CO_2 Reduction
Monday, Oct 30, 8:00 AM
MCC, L100D

Meenesh R. Singh, Chair
Feng Jiao, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

8:00 Welcoming Remarks

8:01 Paper 66a: Understanding Catalyst Selectivity for CO_2 Electro-Reduction
*— **Thomas F. Jaramillo**, Christopher Hahn, Drew Higgins, Jeremy T. Feaster, Stephanie Nitopi, Carlos Morales Guio, Lei Wang, Alan Landers, John Lin, Antaeres Antoniuk-Pablant*

8:19 Paper 66b: Ag-Sn Bimetallic Catalyst with a Core-Shell Structure for CO_2 Reduction
*— Wesley Luc, Charles Collins, **Feng Jiao***

8:37 Paper 66c: Electrochemical CO_2 Reduction over CuAg Bimetallic Electrodes and Well Defined Surface Alloys with Enhanced Oxygenate Selectivity
*— **Ezra L. Clark**, Christopher Hahn, Thomas F. Jaramillo, Alexis T. Bell*

8:55 Paper 66d: A Carbon Nanotube–Supported Gold Catalyst for the Electroreduction of Carbon Dioxide (CO_2)
*— **Sumit Verma**, Yuki Hamasaki, Chaerin Kim, Wenxin Huang, Shawn Lu, Molly Jhong, Tsuyohiko Fujigaya, Naotoshi Nakashima, Paul J. A. Kenis*

9:13 Break

9:17 Paper 66e: Interplay of Mass Transfer and Local pH Effects in CO_2 Reduction Electrocatalysis on Cu Nanowires
*— David Raciti, **Chao Wang***

9:35 Paper 66f: Measurement of Intrinsic Activity of Electrocatalytic Reduction of CO_2 over Cu
*— **Aditya Prajapati**, Meenesh R. Singh*

9:53 Paper 66g: Electrocatalytic Carbon Fixation on Molecular-Functionalized Surfaces
*— **Ming Gong**, Zhi Cao, Wei Liu, Christopher Chang*

10:11 Paper 66h: Electrochemical Reduction of CO_2 on Metal-Doped Graphene
*— Charlotte Kirk, Leanne Chen, **Samira Siahrostami**, Mohammadreza Karamad, Michal Bajdich, Johannes Voss, Jens Nørskov, Karen Chan*

10:29 Concluding Remarks

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(67) Emerging Tools and Enabling Technologies in Synthetic Biology and Metabolic Engineering
Monday, Oct 30, 8:00 AM
MCC, 207A/B

Kang Wu, Chair
Cong T. Trinh, Co-Chair

Sponsored by: Bioengineering

8:00 Paper 67a: Modifying IgG Glycan Profile Using a High-Throughput Multi-Gene Assembly Platform
*— **Christopher Stach**, Tung S. Le, Meghan G. McCann, Xinning Chen, Liang Zhao, Michael J. Smanski, Wei-Shou Hu*

8:18 Paper 67b Synthetic Regulation of Sporulation Genes for Tunable Display of Proteins on Bacterial Spore Surface
*— Jiacheng Wan, Erin Drufva, **Kang Wu***

8:36 Paper 67e: Kinetically Controlled RNA Aptamer Biosensors for High-Throughput Production Phenotype Screening
*— **Cassandra Burke**, James Carothers*

8:54 Paper 67d: Retron-Based Targeted Mutagenesis Enabling In-Vivo Continuous Evolution in *E. coli*
*— **Xiang Zheng**, Tianmin Wang, Xin-Hui Xing, Chunbo Lou, Chong Zhang*

9:12 Paper 67c: ModCell: A Multiobjective Strain Design Platform for Modular Cell Engineering
*— **Sergio Garcia**, Cong T. Trinh*

9:30 Paper 67f: Optimization-Driven Top-Down Synthesis of Genome-Minimized Strains for Bioproduction
*— **Lin Wang**, Costas D. Maranas*

9:48 Paper 67g: Genome-Scale Engineering: A New Frontier in Metabolic Engineering *— **Huimin Zhao***

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(68) Engineering Government Policy with a Chemical Perspective (Invited Talks)
Monday, Oct 30, 8:00 AM
MCC, 101H

Rudra Palash Mukherjee, Chair
Jon Haughton, Co-Chair

Sponsored by:
Young Professionals Committee (YPC)

8:00 Paper 68a: Into Hot Water: Utilizing Thermal Distributed Energy Resources to Improve Grid Reliability
*— **Elena Shanin***

8:25 Paper 68b: Turning the Tide: Policies to Advance Saltwater Desalination in the United States
*— **Lauren Bartels***

8:50 Paper 68c: Microgrids for the Macrogrid: A Policy Framework for the Deployment of Advanced Microgrids
*— **Julia Zhuang***

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(69) Engineering in Cancer Biology and Therapy I
Monday, Oct 30, 8:00 AM
MCC, 208B

Samira M. Azarin, Chair
Shreyas Rao, Co-Chair
Nicholas Graham, Co-Chair

Sponsored by:
Engineering Fundamentals in Life Science

8:00 Paper 69a: Targeting Chemoresistance in Bioengineered 3D Tumor Models: Rationally Designed Combination Therapies Informed by Physical Stress and Heterocellular Communication
*— **Imran Rizvi***

8:18 Paper 69b: Co-Administration of the Tumor-Penetrating Peptide iRGD Improves the Therapeutic Efficacy of Paclitaxel in a 3D Air-Grown Lung Cancer Model
*— **Sweta K. Gupta**, Samantha A. Meenach*

8:36 Paper 69c: Capturing Microenvironmental Regulation of Metastatic Dormancy and Recurrence
*— Ryan Carpenter, Shelly Peyton, **Jungwoo Lee***

8:54 Paper 69d: 3D Organotypic Cancer Model: Pancreatic Ductal Adenocarcinoma Replaces Endothelium During Tissue Invasion
*— **Duc-Huy Nguyen**, Esak Lee, Stella Alimperti, Alec Wong, Jeroen Eyckmans, Ben Stanger, Christopher Chen*

9:12 Paper 69e: Photothermal Therapy of Bladder Cancer via Targeted Single-Walled Carbon Nanotubes
*— Needa Virani, Patrick McKernan, Robert Hurst, Joel Slaton, **Roger Harrison***

9:30 Paper 69f: Sprouty2 Regulates Signaling and Phenotypic Responses of Glioblastoma Cells to DNA Damaging Agents and Receptor Kinase Inhibitors
*— **Nisha G. Sosale**, Matthew J. Lazzara*

9:48 Paper 69g: Function and Regulation of Regenerating Proteins in Pancreatic Cells
*— Fan Zhang, Shawna Downing, Jessica T. Stieglitz, James Van Deventer, **Emmanuel S. Tzanakakis***

10:06 Paper 69h: In-Vitro Model of Breast Cancer Cell Dormancy Under Hypoxia-Mimicking Microenvironments Using Cobalt Chloride
*— **Hak Rae Lee**, Samira M. Azarin*

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(70) Faculty Candidates in CoMSEF I: Biomolecules, Soft Materials, and Algorithms
Monday, Oct 30, 8:00 AM
MCC, L100H

M. Scott Shell, Chair
Amir Haji-Akbari, Co-Chair

Sponsored by:
Computational Molecular Science and Engineering Forum

8:00 Paper 70a: A Generic Coarse-Grained Model of Influenza Budding: What Can We Learn?
*— **Jesper J. Madsen**, John M. A. Grime, Gregory A. Voth*

8:15 Paper 70b: Allosteric Effects of Gold Nanoparticles on Human Serum Albumin
*— **Qing Shao**, Carol K. Hall*

8:30 Paper 70c: Self-Assembly of Proteins: The Role of Shape and Specific Interaction
*— **Jens Glaser,** Sharon C. Glotzer*

8:45 Paper 70d: Predictive Design of Next-Generation Nanomaterials and Devices via Bottom-Up Approaches
*— **Trung Nguyen***

:00 Paper 70e: Solvation of Self-Assembled Complexes: Using Molecular Simulations to Probe Energetics, Structure, and Dynamics
*— **Kevin R. Hinkle**, Frederick R. Phelan Jr.*

9:15 Paper 70f: Level-Set Strategy for Self-Consistent Field Theory
*— **Gaddiel Ouaknin***

9:30 Paper 70g: Simulations of Nonlinear Flows in Nonequilibrium Complex Liquids
*— **Rui Zhang***

9:45 Paper 70h: Employing a Multipole Approximation in a Hybrid Fluid via Relative Resolution
*— **Aviel Chaimovich**, Christine Peter, Kurt Kremer*

10:00 Paper 70i: Effects of Particle Friction on the Fatigue Failure of Granular Materials Under Cyclic Compression *— **Somayeh Farhadi***

10:15 Paper 70j: Quantitatively Reliable Molecular Modeling and Simulation of Vapor-Liquid Equilibria
*— **Martin T. Horsch***

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(71) Forum Plenary: Pharmaceutical Discovery, Development, and Manufacturing Forum (Invited Talks)
Monday, Oct 30, 8:00 AM
MCC, 205A/B

Zoltan K. Nagy, Chair

Sponsored by:
Pharmaceutical Discovery, Development and Manufacturing Forum

8:00 Introduction by Zoltan K. Nagy, Purdue University

8:05 Paper 71a: Automated Systems for Screening, Kinetics, and Optimization of Chemical Synthesis and On Demand Production
*— **Klavs F. Jensen***

8:50 Paper 71b: Can Laboratory Automation Finally Fulfill the Promise of Revolutionizing Pharmaceutical Discovery? *— **Scott Sheehan***

9:35 Paper 71c: Emerging Technology: A Key Enabler for Modernizing Pharmaceutical Manufacturing and Advancing Product Quality
*— **Thomas O'Connor**, Celia N. Cruz, Sau Lee*

TECHNICAL SESSIONS 2017

(72) Fundamentals and Applications of Flow Assurance
Monday, Oct 30, 8:00 AM
MCC, 200B

Francisco Vargas, Chair

Sponsored by:
Upstream Engineering and Flow Assurance Forum

8:00 Paper 72a: Investigation of the Impact of Inorganic Solids on Asphaltenes Precipitation
— ***Yuan Yang***,
Wattana Chaisoontornyotin, Jingzhou Zhang, Samson Ng, Michael P. Hoepfner

8:20 Paper 72b: Microstructure of Asphaltenes in Solvent Blends Investigated by Viscometry
— ***Weiyi Kong***

8:40 Paper 72c: Characterization of Gas Hydrate Slurry Viscosity Using a High-Pressure Rheometer
— ***Ahmad Abdul Majid***, *David T. Wu, Carolyn A. Koh*

9:00 Paper 72d: Avoiding Flowline Plugging: Emulsion+Ice+Wax+Hydrate, the Beast Flow Assurance Discipline Must Confront
— ***Ben Bbosa***, *Amaka Waturuocha, Hongfei Xu, Deepak Monteiro, Sasi Chaganti, Michael Volk*

9:20 Break

9:30 Paper 72e: Mass Transfer During Hydrate Formation in Water-Oil-Gas System
— *Dongdong Guo, Wenjia Ou,* ***Fulong Ning***, *Zhichao Liu, Wanjun Lu, Carolyn A. Koh*

9:50 Paper 72f: Enhancing Hydrate Inhibition Performance of Biomolecules by Doping with Synergents
— ***Majeda Khraisheh Sr.***

10:10 Paper 72g: Investigation on the Effect of Wax on Hydrate Formation Characteristics and Flow Properties in a High-Pressure Flowloop
— ***Yang Liu***, *Bohui Shi, Ye Zhag, Lin Ding, Yu Yong, Shangfei Song, Wei Wang, Jing Gong*

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(73) Fundamentals of Environmental Kinetics and Reaction Engineering
Monday, Oct 30, 8:00 AM
MCC, 102E

Panagiotis Smirniotis, Chair
Victor R. Vasquez, Co-Chair

Sponsored by: Fundamentals

8:00 Paper 73a: Heterogeneous Elemental Mercury Oxidation Kinetics over RuO_2/TiO_2 Catalyst
— ***Zhouyang Liu***, *Vishnu Sriram, Can Li, Joo-Youp Lee*

8:25 Paper 73b: Fundamental Chemistry, Kinetics and Mass-Transfer Aspects of the Emerging Sulfate Radical–Based Environmental Technologies for Pollution Control
— ***Yusuf G. (Debo) Adewuyi***

8:50 Paper 73c: Minimum Ignition Energy Measurement for Explosive Disproportionation of New Refrigerant Trifluoroethylene
— ***Tetsuo Otsuka***, *Katsuya Ueno, Hidekazu Okamoto, Masamichi Ippommatsu, Ritsu Dobashi*

9:15 Paper 73d: Bioremediation of Petroleum-Contaminated Soil Using Three Simultaneously Operated Bioreactors
— ***Mohammad-Saeed Safdari***, *Farhad Fazlollahi, Hamid-Reza Kariminia*

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(74) Fundamentals of Fluidization I
Monday, Oct 30, 8:00 AM
MCC, 200I

Marc-Olivier Coppens, Chair
Mayank Kashyap, Co-Chair

Sponsored by:
Fluidization and Fluid-Particle Systems

8:00 Paper 74a: Understanding Particulate Flow Behavior: Fluidized Bed, Pneumatic Conveying and Membrane Filtration Processes
— ***Jia Wei Chew***

8:17 Paper 74b: CFD-DEM Simulation of the Heat Transport in a Wurster Coater
— ***Peter Böhling***, *Dalibor Jajcevic, Johannes G. Khinast*

8:34 Paper 74c: Development of a Rheological Model for Cohesive Granular Materials Across Dense and Dilute Flow Regimes
— *Yile Gu, Ali Ozel,* ***Sankaran Sundaresan***

8:51 Paper 74d: CFD-DEM Simulations of Bubbling Fluidization: Global Sensitivity Analysis for the Identification and Validation of Critical Model Parameters
— ***Akhilesh Bakshi***, *Mehrdad Shahnam, Tingwen Li, Christos Altantzis, Aytekin Gel, William A. Rogers, Ahmed F. Ghoniem*

9:08 Paper 74e: The Role of Particle Friction in the Stabilization of Pulsed Gas-Solid Fluidized Beds: From Surface Waves to Structured Bubble Nucleation
— ***Victor Francia***, *Kaiqiao Wu, Lilian de Martín, Marc-Olivier Coppens*

9:25 Paper 74f: Critical Comparison of Electrostatic Effects on Hydrodynamics, Heat Transfer and Chaotic Analysis in a Bubbling Fluidized Bed with a Central Jet
— *Haotong Wang, Musango Lungu, Zhengliang Huang, Jingdai Wang, Yongrong Yang,* ***Qiang Shi***

9:42 Paper 74g: Verification of Euler-Lagrange and Euler-Euler Simulations of Meso-Scale Gas-Solid Flows
— *Ravi G. Patel,* ***Bo Kong***, *Jesse Capecelatro, Rodney O. Fox, Olivier Desjardins*

9:59 Paper 74h: Fundamental Prediction of Agglomeration and Entrainment Rates for Cohesive Powders in a Riser Flow
— ***Kevin M. Kellogg***, *Peiyuan Liu, Casey Q. LaMarche, Christine M. Hrenya*

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(75) Gene Regulation Engineering
Monday, Oct 30, 8:00 AM
MCC, 208A

Chase L. Beisel, Chair
Tae Seok Moon, Co-Chair

Sponsored by: Bioengineering

8:00 Paper 75a: Construction of Genetic Devices by Engineering Transcriptional Interference
— ***Antoni E. Bordoy, Anushree Chatterjee***

8:18 Paper 75b: Optogenetic Control of Gene Expression for Metabolic Engineering
— *Evan Zhao, Jared Toettcher,* ***Jose L. Avalos***

8:36 Paper 75c: Establishment of an Artificial Dynamic Regulatory Network and Its Application in Metabolic Engineering
— ***Yaping Yang***, *Yuheng Lin, Jian Wang, Yifei Wu, Ruihua Zhang, Mengyin Cheng, Qipeng Yuan, Yajun Yan*

8:54 Paper 75d: Using Promoter Architecture to Guide Engineering of Strong Fatty Acid Inducible Hybrid Promoters in *Yarrowia lipolytica*
— ***Murtaza Shabbir Hussain***, *Ian Wheeldon, Mark Blenner*

9:12 Paper 75e: A Dual-Acting sRNA of *E. coli* Is Repurposed as a Genetically Portable Metabolic Engineering Controller
— *Samuel D. Stimple, Ashwin Lahiry, Hopen Yang, David W. Wood,* ***Richard A. Lease***

9:30 Paper 75f: Design and Characterization of Orthogonal Pol II gRNA Expression Systems for dCas9 Transcriptional Repression Networks in *s. cerevisiae*
— ***William Voje Jr.***, *Miles W. Gander, Justin Vrana, Eric Klavins, James Carothers*

9:48 Paper 75g: Uncovering How RNA Molecules 'Make Decisions' on the Fly: Towards Understanding and Engineering Cotranscriptional RNA Folding
— ***Julius B. Lucks***

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(76) In Honor of Martin Yarmush I (Invited Talks)
Monday, Oct 30, 8:00 AM
MCC, 208C/D

Kyongbum Lee, Chair
Arul Jayaraman, Co-Chair

Sponsored by:
Food, Pharmaceutical & Bioengineering Division

8:00 Paper 76a: Overcoming Oxygen Supply Limitations in Islet Transplantation
— ***Clark K. Colton***

8:22 Paper 76c: Invited Talk
— ***Mehmet Toner***

8:44 Paper 76d: The Amyloid Regulatory Network Hypothesis
— ***Regina M. Murphy***

9:06 Paper 76e: Invited Talk
— ***David Odde***

9:28 Paper 76f: Invited Talk
— ***David A. Kofke***

9:50 Paper 76g: Invited Talk
— ***Francois Berthiaume***

10:12 Paper 76b: Linking Cancer and Metabolism via Isotope Labeling and Network Analysis
— ***Gregory N. Stephanopoulos***

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(77) In Honor of the 2016 Wilhelm Award Winner I (Invited Talks)
Monday, Oct 30, 8:00 AM
MCC, L100A

John R. Regalbuto, Chair
Jonas Baltrusaitis, Co-Chair
Israel E. Wachs, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

8:00 Paper 77a: Climbing Elementary Steps to the Pinnacle: Surface Science to Heterogeneous Catalysis
— ***Robert J. Madix***

8:25 Paper 77b: Catalyst Synthesis by Atomic Layer Deposition
— ***Peter C. Stair***

8:50 Paper 77c: Single-Site or Not Single-Site?
— ***Christophe Copéret***

9:15 Paper 77d: Promotion of Platinum for Alkane Dehydrogenation: Intermetallic Alloys with Two Catalytically Active Metals
— *Laryssa Cesar, Evan Wegener, Zhenwei Wu,* ***Jeffrey T. Miller***

9:40 Paper 77e: Challenges with Model Catalysts — ***Mark Barteau***

10:05 Paper 77f: Nature of Active Selective Oxidation Catalysts: an Operando Approach
— ***Robert Schlogl***

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(78) Materials for Electrochemical Energy I
Monday, Oct 30, 8:00 AM
MCC, 210A/B

Gang Wu, Chair
Juchen Guo, Co-Chair
Aaron T. Fafarman, Co-Chair

Sponsored by:
Electronics and Photonics

8:00 Paper 78a: Solid Dispersions of Electroactive Materials for Energy Storage Applications
— ***Gary M. Koenig Jr.***, *Zhaoxiang Qi, Devanshi Gupta*

8:22 Paper 78b: Rational Design of the Cathode Materials in the Lithium-Sulfur Batteries
— ***Tong Mou***, *Bin Wang*

8:38 Paper 78c: 3D Carbon Materials for Electric Double-Layer Capacitors with Ultrahigh Areal Capacitance
— ***Liang Chang***, *Yun Hang Hu*

8:54 Paper 78d: 3D High-Surface-Area and Mesoporous Graphene Sheet-Like Carbon for Supercapacitors
— *Haiyang Shen, Min Wei,* ***Gang Wu***

9:10 Paper 78e: Stability Predictions for Dimethoxybenzene-Based Catholyte Materials — ***Benjamin Silcox***, *Rajeev Assary, Jing Jing Zhang, Siu on Tung, Ilya Shkrob, Lu Zhang, Levi T. Thompson*

9:26 Paper 78f: Solvate Ionic Liquid-Based Gel Electrolytes Containing Functionalized Polymer-Based Networks for Use in Lithium-Metal Battery Applications
— *Anthony D'Angelo, Matthew J. Panzer*

9:42 Paper 78g: Studies on Complex Electrolytes for Magnesium Batteries
— *Laura Merrill, Hunter Ford,* ***Jennifer Schaefer***

9:58 Paper 78h: First-Principles Study of Temperature Dependence of Energy Gaps in Gas Sensor Materials
— ***Yuning Wu***, *Yuhua Duan, Paul R. Ohodnicki, Benajmin T. Chorpening*

10:14 Paper 78i: Supercritical Fluid-Based Synthesis of Antimony Electrode Materials
— *Grant A. Williamson, Elena P. Pandres,* ***Vincent C. Holmberg***

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(79) Materials Innovations Inspired by Acrivos Award Winner Chris Jones II
Monday, Oct 30, 12:30 PM
MCC, 211A

Nicholas Brunelli, Chair
Jason C. Hicks, Co-Chair

Sponsored by:
Materials Engineering and Sciences Division

12:30 Paper 79a: Tuning the Molecular Design of Catalytic Materials to Increase Activity and Selectivity for Fine Chemical Production
— ***Nicholas Brunelli***, *Aamena Parulkar, Nitish Deshpande, Mariah Whitaker, Rutuja Joshi*

12:47 Paper 79b: Deactivation of Zeolite Catalysts During Hydrodeoxygenation of Aromatic Oxygenates — *Guo Shiou Foo, Mariana V. Rodrigues, Qandeel Almas, Chukwuemeka Okolie, Matt Yung,* ***Carsten Sievers***

1:04 Paper 79c: Improving Methanol-to-Olefins Conversion Performance of CHA Materials by Seeding the Hydrocarbon Pool
— ***Praveen Bollini***, *Aditya Bhan*

1:21 Paper 79d: Tuning of Higher Alcohol Selectivity and Productivity in CO Hydrogenation Reactions over K/MoS_2 Catalysts Supported on Mesoporous Activated Carbon and Mixed MgAl Oxide
— ***Micaela Taborga Claure***, *Song-Hai Chai, Sheng Dai, Faisal M. Alamgir, Pradeep K. Agrawal, Christopher W. Jones*

1:38 Paper 79e: Kinetic and Spectroscopic Investigations of Alcohol Conversions over Metal Oxide Catalysts
— ***Shuai Tan***, *Yongqiang Cheng, Luke L. Daemen, Ho Nyung Lee, Benjamin Doughty, Daniel Lutterman*

1:55 Paper 79f: Catalytic Upgrading of Fast-Pyrolysis Bio-Oil for Renewable Hydrocarbon Production
— ***Mariefel V. Olarte***, *Huamin Wang, Daniel M. Santosa, John G. Frye, Suh-Jane Lee, Jae-Soon Choi, Pimphan Aye Meyer, Susanne Jones, Corinne Drennan, Alan H. Zacher*

2:12 Paper 79g: Chemical Reaction Engineering Principles of Continuous-Flow Photoredox Catalysis
— ***Eric G. Moschetta***, *Kaid Harper, Steve Richter, Steven J. Wittenberger*

2:29 Paper 79h: Factors Affecting Catalytic Performance in the Presence of Non-Thermal Plasmas
— *Jongsik Kim, Prateek Mehta, Patrick Barboun, William Schneider, David Go,* ***Jason C. Hicks***

2:46 Paper 79i: Accelerating Innovation in Advanced Manufacturing
— ***Michael McKittrick***

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(80) Materials Synthesis and Processing with Compressed or Supercritical Fluids
Monday, Oct 30, 8:00 AM
MCC, M100C

Christopher L. Kitchens, Chair

Sponsored by: High Pressure

8:00 Paper 80a: Production of High-Purity Pyrene Oligomers in a Supercritical Fluids Medium
— ***Willam Lamie***, *Mark C. Thies**

8:20 Paper 80b: Development and Analysis of Green Pathways Isolation of Medically Active Components from Grape Pomace Biomass
— ***Kyle Cogswell***, *Aydin K. Sunol*

8:40 Paper 80c: A Novel Supercritical CO_2-Based Treatment for Decellularization That Maintains Mechanical and Structural Integrity
— *Dominic M. Casali, Rachel M. Handleton,* ***Michael A. Matthews***

9:00 Paper 80d: Supercritical Fluid–Enhanced Swelling and Drug Impregnation of Biomedical Polymers
— ***Kyle Cogswell***, *Aydin K. Sunol*

9:20 Paper 80e: Effect of Precursor on Crystal Structure of Titania Synthesis in Supercritical Sol-Gel Reaction
— ***Motohiro Kinoshita***, *Yusuke Shimoyama*

9:40 Paper 80f: Accelerated Conversion of Magnesium Oxychloride to Chlorartinite Using Pressurized Carbon Dioxide and the Resulting Increased Water Resistance
— ***Roque Góchez, Christopher L. Kitchens***, *Thomas Vreeland*

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(81) Microfluidic and Nanoscale Flows: Separations & Particulates
Monday, Oct 30, 8:00 AM
Hilton, Conrad D

Siva A. Vanapalli, Chair
Cari S. Dutcher, Co-Chair

Sponsored by: Fluid Mechanics

8:00 Paper 81a: High-Throughput Mechanical Stimulation and Functional Imaging *In Vivo* — ***Hang Lu***

8:30 Paper 81b: The Steady Motion of a Train of Vesicles in a Cylindrical Channel of Arbitrary Cross Section
— ***Joseph M. Barakat***, *Eric S. G. Shaqfeh*

8:45 Paper 81c: The Dissolution of a Sheared Water Drop in Bitumen Measured Using a Novel Microfluidic Platform
— ***Sachin Goel***, *Samson Ng, Edgar Acosta, Arun Ramachandran*

9:00 Paper 81d: Adhesion and Breakup of Model Metastatic Cancer Cell Clusters During Passage Through a Microfluidic Constriction
— ***Yeng-Long Chen***, *Sam Au, Mehmet Toner*

9:15 Paper 81e: Chaotic Thermal Convection in Microfluidic Hydrothermal Pore Environments
— *Aashish Priye, Yuncheng Yu, Vijay Ravisankar, Yassin A. Hassan,* ***Victor M. Ugaz***

9:30 Paper 81f: Using Droplet Microfluidics to Study Chemical Thermodynamics of Aqueous Atmospheric Aerosol Particles
— ***Lucy Nandy***, *Cari S. Dutcher*

9:45 Paper 81g: Analysis of the Engulfment of a Foreign Particle by a Solidification Interface: A New Scaling for Flow and Interfacial Forces Involving SiC Particles During Silicon Crystal Growth — ***Jeffrey J. Derby***, *Yutao Tao, Christian Reimann, Jochen Friedrich, Thomas Jauss, Tina Sorgenfrei, Arne Croell*

10:00 Paper 81h: Hydrodynamic Mobility of Particles, Vesicles and Cancer Cells in a Square Microchannel
— ***Shamim Ahmmed***, *Naureen Suteria, Valeria Garbin, Siva A. Vanapalli*

10:15 Paper 81i: Deformable Droplet Migration in a Narrow Microchannel at Finite Reynolds Numbers via Dissipative Particle Dynamics (DPD)
— ***Ryan L. Marson***, *Ronald G. Larson*

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(82) Modeling and Analysis of Chemical Reactors
Monday, Oct 30, 8:00 AM
MCC, L100E

Anthony G. Dixon, Chair
Sanjeev M. Rao, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

8:00 Paper 82a: Experimental and Modeling Studies of Cycle Frequency, Reductant Type and Non-Isothermal Effect on the Performance of a Lean NO_x Trap
— ***Allen Wei-Lun Ting***, *Vemuri Balakotaiah, Michael Harold*

8:20 Paper 82b: Fast Optimal Control of Exothermic Packed-Bed Reactors via Reduced-Order Models
— ***Jens Bremer***, *Peter Benner, Kai Sundmacher*

TECHNICAL SESSIONS 2017

8:40 Paper 82c: From Particle-Resolved CFD to the Transient Modeling of Dynamic Systems: Dispersion in Fixed-Bed Reactors
*— **Nico Jurtz**, Philipp Waldherr, Gregor D. Wehinger, Matthias Kraume*

9:00 Paper 82d: N-Butane Partial Oxidation in a Fixed Bed: A Local Selectivity Study by Detailed Numerical Simulations
*— **Behnam Partopour**, Anthony G. Dixon*

9:20 Paper 82e: Bifurcation Analysis for Allothermic High-Temperature Pyrolysis of Methane in a Moving-Bed Reactor
*— David W. Agar, Alejandro A. Munera Parra, **Frank Platte***

9:40 Paper 82f: Catalytic Membrane Reactor for CO_2 Hydrogenation Using H_2-Containing Renewable Streams: Model-Based Feasibility Analysis
*— Robert Currie, **David Simakov***

10:00 Paper 82g: Experimental and Modeling Studies of Residence Time Distribution in Partially Filled Laminar-Flow Reactors
*— **Sundari Ramji**, Anil Vir, S. Pushpavanam*

(83) Modeling of Interfacial Systems
Monday, Oct 30, 8:00 AM
MCC, M100A

Ateeque Malani, Chair
Ketan S. Khare, Co-Chair
Patricia Taboada-Serrano, Co-Chair

Sponsored by: Interfacial Phenomena

8:00 Welcoming Remarks

8:03 Paper 83a: Using Molecular Simulation to Understand the Interfacial Behavior of Ionic Liquids
*— Xiaoyu Liang, **Jeffrey R. Errington***

8:21 Paper 83b: Capacitance and Ion Dynamics of Ionic Liquids near Oxidized Graphene
*— **Yu Zhang**, Boris Dyatkin, Yury Gogotsi, Peter T. Cummings*

8:39 Paper 83c: Using Simulations and Experiments to Characterize Water Structure near Mica Surfaces for Heterogeneous Ice Nucleation
*— Brittany Glatz, Jiarun Zhou, **Sapna Sarupria***

8:57 Paper 83d: A Novel Density Gradient Theory for Surfactant Molecules Applied to Oil/Water Interfaces
*— **Xiaoqun Mu**, Walter G. Chapman*

9:15 Paper 83e: Computational Chemistry Design of Liquid Crystal–Based Chemoresponsive Systems with Increased Water Tolerance
*— **Tibor Szilvási**, Huaizhe Yu, Prabin Rai, Robert Twieg, Nicholas L. Abbott, Manos Mavrikakis*

9:33 Paper 83f: Thin Liquid Film Stability in Various Interaction Regimes Arising Due to Surface Active Agents
*— Paidi Venkatesh Kumar, U Hariharan, Anjishnu Choudhury, Harish N. Dixit, **Sreeram K. Kalpathy***

9:51 Paper 83g: A Semi-Empirical Analytical Model for Determining the Thermodynamic Stability of Pickering Emulsion
*— **Guolin Zhao**, Junyin Xiao, Yanyang Wu, Shuangliang Zhao Sr., Honglai Liu*

10:09 Paper 83h: Computational Method for Extracting Individual Adsorption Parameters from Experimental Dynamic Interfacial Tension of Mixed Surfactant Solutions
*— **Fang Liu**, Nelya Akhmetkhanova, Vincent Pauchard*

10:27 Concluding Remarks

(84) Molecular Simulation of Surface, Interface and Confinement Effects — In Honor of Keith Gubbins's 80th Birthday I (Invited Talks)
Monday, Oct 30, 8:00 AM
MCC, L100I

Liangliang Huang, Chair
Erik E. Santiso, Co-Chair
Francisco R. Hung, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

8:00 Paper 84a: Atomistic Simulations of Ordered and Disordered Carbons: "Mimicking" Versus "Targeting"
*— **Roland J.-M. Pellenq***

8:19 Paper 84b: Graphene Oxide Membranes: A Molecular Simulation Approach
*— Christopher Williams, Paola Carbone, **Flor R. Siperstein***

8:38 Paper 84c: Polyethylene Oxide (PEO) in a Polyethylene (PE) Framework: A Simple Model for Simulation Studies of Scaling and Solvent Effects on Polymers in an Open Framework
*— **Kwong-Yu Chan**, Liangxu Xie, Nicholas Quirke*

8:57 Paper 84d: Molecular Understanding and Design of Zwitterionic Materials
*— **Shaoyi Jiang***

9:16 Paper 84e: Interfacial Transport of Protons on a 2-Dimensional Functionalized Graphane Surface
*— **J. Karl Johnson**, Abhishek Bagusetty, Bridget Derksen, Pabitra Choudhury*

9:35 Paper 84f: Gas Adsorption Behavior in Ionic Polyimide Composite Membranes
*— **C. Heath Turner**, Asghar Abedini, Ellis Crabtree, Jason E. Bara*

9:54 Paper 84g: Computational Simulation of Supported Nanocatalysts Under Realistic Conditions
*— **Jian-guo Wang***

(85) Nanomaterials for Biological Applications I
Monday, Oct 30, 8:00 AM
MCC, 200G

Anushree Chatterjee, Chair
Prashant Nagpal, Co-Chair

Sponsored by: Nanomaterials for Applications in Energy and Biology

8:00 Paper 85a: Point-of-Care Diagnostics: Nanostructured Materials for Electrochemical Biosensing
*— **Sahar S. Mahshid***

8:25 Paper 85b: Self-Assembling Nanoparticles for Peptide Delivery with Enhanced Stability
*— **Handan Acar**, Mathew R. Schnorenberg, James L. LaBelle, Matthew V. Tirrell*

8:50 Paper 85c: Block Copolymer Nanoparticle for Biofilm Dispersal of Gram-Positive MRSA and VRE
*— **Mary B. Chan-Park**, Jianghua Li*

9:15 Paper 85d: Genetically Targeted Brain-Machine Interface
*— **Jia Liu**, Ariane Tom, Fikri Birey, Charu Ramakrishnan, Sergiu P. Pasca, Zhenan Bao, Karl Deisseroth*

9:40 Paper 85e: Colorimetric Detection of Nitrite Ions Based on the Aggregation of Gold Nanoparticles
*— Aniruddha Kulkarni, Victoria Bird, **Kirk J. Ziegler***

10:05 Paper 85f: Cancer Cell Hyperactivity and Membrane Dipolarity Monitoring via Raman Mapping of Interfaced Graphene: Towards Non-Invasive Cancer Diagnostics
*— Bijentimala Keisham, Arron Cole, Phong Nguyen, Ankit Mehta, **Vikas Berry***

(86) Novel Catalytic and Separation Process Based on Ionic Liquids
Monday, Oct 30, 8:00 AM
MCC, 103A

Zhang Suojiang, Chair
Dickson E. Ozokwelu, Co-Chair

Sponsored by: Innovations of Green Process Engineering for Sustainable Energy and Environment

8:00 Paper 86a: Adsorption of Polar Molecules onto Electrodes Driven by the Combined Effects of Dielectric Inhomogeneity and Electrostatic Correlation
*— **Hongbo Chen**, Issei Nakamura*

8:17 Paper 86b: Extraction of Carboxylic Acid from Aqueous Solution by Strong Hydrogen Bond Basicity Ionic Liquids
*— Yinge Bai, **Ruiyi Yan**, Jianguo Qian, Xiangping Zhang, Suojiang Zhang*

8:34 Paper 86c: Unlocking Biomass Recalcitrance Using Lignin-Based Ionic Liquids
*— **Ning Sun**, Yebon Lee, Ling Liang, Qian He, Roland Kalb, David Blauch, Todd Pray, Aaron Socha*

8:51 Paper 86d: Ionic Liquids–Based Consolidated Bioprocessing for Biofuel Production from Lignocellulosic Biomass
*— **N.V.S.N. Murthy Konda, Suojiang Zhang***

9:08 Paper 86e: A Novel Coarse-Grained Model with Explicit Hydrogen Bond for Imidazolium-Based Ionic Liquids
*— **Feng Huo**, Jiahuan Tong, Suojiang Zhang*

9:25 Paper 86f: Efficient Synthesis of Cyclic Carbonates from Atmospheric CO_2 Using a Positive Charge Delocalized Ionic Liquid Catalyst
*— **Zhiguo Zhang***

9:42 Paper 86g: New Catalytical System in Ionic Liquid for Small-Molecule Conversion *— **Zhe Wang***

9:59 Paper 86h: Ionic Liquids for Separation of Aromatics and Aliphatics: Extraction and Regeneration of Solvent Using CO_2
*— **Michael J. Lubben**, Joan F. Brennecke*

10:16 Paper 86i Ionic Liquids for Absorption and Separation of Gases: An Extensive Database and a Systematic Screening Method
*— **Zhang Suojiang**, Rafiqul Gani*

(87) Novel Mixer and Mixed Reactor Design
Monday, Oct 30, 8:00 AM
MCC, 102D

Sanja Miskovic, Chair
Laura J. Dietsche, Co-Chair

Sponsored by: North American Mixing Forum

8:00 Paper 87a: 3D Printing Through Chaotic Mixing
*— **Grissel Trujillo-de Santiago**, Mario M. Alvarez, Mohamadmahdi Samandari, Gyan Prakash, Gouri Chandrabhatla, Byambaa Batzaya, Pamela Inés Sánchez Rellstab, Alejandro Vallejo-Arroyo, Nasim Annabi, Yu Shrike Zhang, Ali Khademhosseini*

8:19 Paper 87b: Improved Mixing in a Pressure-Driven Straight Microchannel Using Electroosmosis
*— **T. Krishnaveni**, T. Renganathan, S. Pushpavanam*

8:38 Paper 87c: Study of Residence Time Distribution in a Taylor-Couette Reactor *— **Haoyu Wang**, Anh N. Phan, Vladimir Zivkovic, Kamelia Boodhoo*

8:57 Paper 87d: Experimental Investigation of a New Taylor-Couette Cell Design with Radial Fluid Injection for Controlled Mixing Applications
*— **Nikolas A. Wilkinson**, Cari S. Dutcher*

9:16 Paper 87e: Experimental Investigation of PVA–Borax Gel Reaction Flow and Mixing in a Non-Element Mixer
*— **Masaki Yamaguchi**, Takeshi Yokomori, Toshihisa Ueda*

9:35 Paper 87f: Industrial Photo-Chemistry in Agitated Reactors
*— **Werner Himmelsbach**, Rui Soares*

9:54 Paper 87g: Characterizing Mixing Processes Using Computational Fluid Dynamics and z-Transform
*— **De-Wei Yin**, Suraj Deshpande, Sarat Chandra Kuchibhatla*

10:13 Paper 87h: Reactive Mixing in a Stirred-Tank Reactor
— Mahsa Taghavi, Jafarsadegh Moghaddas

(88) Physical Properties for Chemical Process and Product Design
Monday, Oct 30, 8:00 AM
MCC, 102B

Sitaraman Krishnan, Chair
Kenneth R. Cox, Co-Chair

Sponsored by: Product Design

8:00 Introductory Remarks

8:03 Paper 88a: Design Principles for Graphene-Based Materials to Enhance Supercapacitor Performance
*— **Eunsu Paek***

8:26 Paper 88b: Property Model-Based Chemical Substitution and Chemical Formulation Design
*— **Spardha Jhamb**, Xiaodong Liang, Amol Hukkerikar, Kim Dam Johansen, Rafiqul Gani*

8:49 Paper 88c: The Chemical Product Design of Solvents for Post-Combustion CO_2 Capture Processes
*— **Kevin G. Joback**, J. R. Heberle, Abhoyjit S. Bhown*

9:12 Paper 88d: The Effect of Reactor Geometry on Polymer Composition Broadening
*— **Pradeep Jain**, Ivan Konstantinov, Karjala Tom, Carlos Villa*

9:35 Paper 88e: Parameter Estimation of Nonlinear Stochastic Models: Reactivity Ratio Studies in Copolymerization *— **Yuncheng Du***

9:58 Paper 88f: Characterization and Processing of Khulays Clay for Drilling Fluid Application
*— **Jimoh K. Adewole**, Abdullah S. Sultan, Lionel Foganga, Mohamed Mahmoud*

(89) RAPID Process Intensification Institute Update
Monday, Oct 30, 8:00 AM
MCC, 101E

James Bielenberg, Chair

Sponsored by: Process Intensification & Modular Chemical Processing

8:00 Paper 89a: Introductory Remarks
*— **Jim Bielenberg***

8:20 Paper 89a: Autothermal Pyrolysis of Lignocellulose Wastes to Sugars and Other Biobased Products
*— **Robert Brown***

8:40 Paper 89b: Dynamic Process Intensification
*— **Michael Baldea***

9:00 Paper 89c: Manufacturing Supply Chain Development for Solar Thermochemical Modules
*— **Brian Paul,** Somayeh Pasebani, Brian Fronk, Kijoon Lee, Milad Ghayoor, Robert Wegeng, Ward TeGrotenhuis, Richard Zheng and Daryl Brown*

9:20 Paper 89d: Modeling Best Practices Applied to RAPID Assessments *— **Chau-Chyun Chen***

9:40 Paper 89e: Adsorptive Nitrogen Rejection from Natural Gas
*— **Krista Walton,** James Bielenberg, Yang Luo*

10:00 Paper 89f: RD&D Needs for Sustainable Separations
*— **Robert Giraud***

10:20 Concluding Remarks

(90) Reactions in Near-Critical and Supercritical Fluids
Monday, Oct 30, 8:00 AM
MCC, L100B

Keith W. Hutchenson, Chair
Amrit Jalan, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

8:00 Break

8:25 Paper 90b: Continuous Synthesis of Ethyl Esters from Free Fatty Acids over Metal Oxides in Sub-/Supercritical Ethanol
*— **Jiuxu Liu**, Yue Nan, Lawrence L. Tavlarides*

8:50 Paper 90c: Denitrogenation of Pyridine with Acetic Acid as Hydrogen Source Under Catalytic Hydrothermal Gasification Environment
*— **Peng Zhang**, Young Hwan Shin, Lance Schideman, Yuanhui Zhang, Wan-Ting Chen*

9:15 Paper 90d: The Non-Catalytic Decomposition of Lignin into Chemical and Fuel Intermediates
*— **Sara Pourjafar**, Wayne S. Seames*

9:40 Paper 90e: Hydrothermal Liquefaction of Food Waste and Remediation of Aqueous Byproducts
*— **Alex D. Paulsen**, Alex Maag, Ted J. Amundsen, Michael T. Timko, Paul E. Yelvington*

10:05 Paper 90f: Hydrothermal Liquefaction of Wastewater Treatment Microalgae in a Pilot-Scale Continuous-Flow Reactor
*— **Feng Cheng**, Travis Le-Doux, Brian Treftz, Scott Woolf, Juanita Miller, Umakanta Jena, Catherine E. Brewer*

(91) Risk Reduction in and Implementation of Process & Technology Development
Monday, Oct 30, 8:00 AM
MCC, 102C

John Peragine, Chair
Ahmed A. Youssef, Co-Chair
Sergio Mohedas, Co-Chair
Kuang-yao Brian Peng, Co-Chair

Sponsored by: Technology Transfer and Manufacturing

8:00 Paper 91a: Multi-Objective Optimization for Optimal ORC (Organic Rankine Cycle) Design Considering Inherent Risk, Exergy Efficiency
*— **Younggeun Lee**, Seeyub Yang, Kyeongsu Kim, Usama Ahmed, Changsoo Kim, Jeongnam Kim, Chonghun Han*

8:25 Paper 91b: A Study on the Explosion Characteristics in Blast Test Facility by Flammable Gas
*— **Hye-Ri Gye**, Kee Bong Yoon, Chul-Jin Lee*

8:50 Paper 91c: Experimental Safety Plan (ESP) for Safety Management in Chemical Engineering Research
*— **Juanita Miller**, David Rockstraw, Martha Mitchell, Derrik Wootton*

9:15 Paper 91d: Risk Mitigation in Technology Commercialization: Responsibilities of the Owner, Designer and EPC Contractor *— **Kevin Drumm***

9:40 Paper 91e: A Datacentric Approach to Develop Process Design Packages Destined for Mega Projects
*— **Jasmeer Ramlal**, Sergio Mohedas, Xi Chen, Minghua Ye*

10:05 Paper 91f: Transfer of Critical Technology Learnings and Unknown to the Engineering Design Package
*— **Jack Dever***

(92) Soft Matter Hydrodynamics
Monday, Oct 30, 8:00 AM
Hilton, Marquette I/II/III/VIII/IX

James Swan, Chair
Anson Ma, Co-Chair

Sponsored by: Fluid Mechanics

8:00 Paper 92a: The Importance of Classical Soft Matter Physics in the Development of New Nanomaterials
*— **Matteo Pasquali***

8:30 Paper 92b: Rapid and Accurate Methods for Modeling Hydrodynamic Forces in Brownian Dynamics Simulations
*— **Andrew Fiore**, James Swan*

8:45 Paper 92c: Rotational Dynamics of Nanoparticles in Polymer Solutions and Melts
*— Lorena Maldonado-Camargo, **Carlos Rinaldi***

9:00 Paper 92d: Morphology of Nanoparticle Aggregates in Flow Through Beds Packed with Spheres: Self- and Flow-Induced Assembly Using Lattice Boltzmann Simulations
*— **Ngoc Hong Pham**, Dimitrios V. Papavassiliou*

9:15 Paper 92e: Shear Thickening of Colloidal Dispersions at High Particle Concentrations: Rheology and SANS Investigations into Particle-Scale Mechanisms
*— Kevin Whitcomb, **Norman Wagner***

9:30 Paper 92f: Colloidal Hydrodynamics at a Fluid-Fluid Interface
*— **Charles Maldarelli**, Archit Dani*

9:45 Paper 92g: Effect of Surface Geometry on the Frictional Properties of Poly(dimethyl siloxane)
— ***Yunhu Peng***, *Lilian Hsiao*

10:00 Paper 92h: Microrheology and Structural Reconfiguration of Artificial Biofluids Composed of Xanthan Gum in Salt Solutions
— *Mingyang Tan, Yating Mao, Britany M. Swann,* ***Travis W. Walker***

10:15 Paper 92i: Probe Rheology Simulation Technique for Determination of Viscoelasticity of Complex Fluids
— ***Pouria Nourian***, *Dinesh Sundaravadivelu Devarajan, Rajesh Khare*

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(93) Solid-Liquid Interfaces
Monday, Oct 30, 8:00 AM
MCC, M100B

Kai Kristiansen, Chair
Ateeque Malani, Co-Chair
Jing Yu, Co-Chair

Sponsored by: Interfacial Phenomena

8:00 Paper 93a: Approach to Contact, and Adhesion at Elastic and Structured Interfaces — ***Joelle Frechette***

8:15 Paper 93b: Competitive Adsorption of Ions at Solid-Liquid Interface: Molecular Simulation Study
— ***Sai Krishna Reddy Adapa,*** *Ateeque Malani*

8:30 Paper 93c: Surface Modification of Stainless Steels for Advanced Functionalities
— ***Won Tae Choi***, *Victor Breedveld, Dennis W. Hess, Preet M. Singh*

8:45 Intermission

8:50 Paper 93d: Understanding the Wetting Behavior of Water-Octane-Silica Systems Using Monte Carlo Simulation
— *Wenjing Guo,* ***Jeffrey R. Errington***

9:05 Paper 93e: Time-Resolved In-Situ Studies of Zeolite Crystal Growth
— ***Madhuresh K. Choudhary***, *Manjesh Kumar, Jeffrey D. Rimer*

9:20 Paper 93f: Understanding the Solid-Liquid Phase Transition During the Growth of Scintillator Single Crystals via Computational Modeling and Neutron Imaging
— ***Chang Zhang***, *Jeffrey H. Peterson, Jan Seebeck, Anton S. Tremsin, Didier Perrodin, Gregory A. Bizarri, Edith D. Bourret, Sven Vogel, Jeffrey J. Derby*

9:35 Break

9:40 Paper 93g: Efficient Dispersion of Crude Oil by Blends of Food-Grade Surfactants: Toward Greener Oil Spill Treatments
— *David Riehm, Jasmin C. Athas, John Neilsen, Geoffrey D. Bothun, Vijay T. John, Srinivasa R. Raghavan,* ***Alon McCormick***

9:55 Paper 93h: Comparison of Experimental and Predicted Adsorption Isotherms of Mixtures
— ***Julian Butz***, *Sabine Enders*

10:10 Paper 93i: Towards Connecting the Microstructural and Structural Changes in Hierarchical Nanoporous Materials (e.g., Clays) During Gas Adsorption (CO_2, CH_4, H_2) Using In-Operando Multiscale X-Ray and Neutron Scattering Measurements
— ***Greeshma Gadikota***, *Andrew J. Allen*

10:25 Concluding Remarks

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(94) Sustainable Energy from Renewable Resources
Monday, Oct 30, 8:00 AM
MCC, 101C

Hanieh Niroomand, Chair
Vikas Khanna, Co-Chair
Emre Gençer, Co-Chair

Sponsored by: Sustainable Energy

8:00 Paper 94a: Producing Biocrude from Renewable Feedstocks Through Hydrothermal Liquefaction
— ***Yanna Liang***, *Zheting Bi, Ji Zhang, Zeying Zhu, Tomasz Wiltowski*

8:17 Paper 94b: Cell Lysis, Lipid Recovery, and Lipid Hydroprocessing from Oleaginous Yeast
— ***Jacob S. Kruger***, *Nicholas Cleveland, RouYi Yeap, Tao Dong, Nicholas J. Nagle, Gregg T. Beckham, James D. McMillan, Mary Biddy*

8:34 Paper 94c: Wood Pellet Boiler Heating Systems Evaluation and Optimization — ***Kui Wang***, *Philip K. Hopke, Marco Satyro*

8:51 Paper 94d: An MILP Model for Integrated Carbon-Free Heat Networks Considering Alternative Energy Vectors
— ***André Prates Pereira***, *Sheila Samsatli*

9:08 Paper 94e: Characterization of Used Cooking Oils and Their Supply Chain for the Exploitation as Raw Materials in Urban Biorefineries
— ***Luz Angela Rincón Vija***, *Alvaro Orjuela, Paulo Cesar Narváez Rincón, Juan Guillermo Cadavid*

9:25 Paper 94f: Electrochemical Activity of Non-Noble Metal Alloy as Catalyst Towards Oxidation of Glycerol in Acidic Media: A Case for the Conceptual Glycerol/Ferric Redox Flow Battery — ***James Akrasi***

9:42 Paper 94g: Fecralloy Catalysts Partially Oxidize Methane to Syngas Selectively — *Zhenni Ma, Diego C. Pelegrin, Daria C. Boffito,* ***Gregory S. Patience***

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(95) Sustainable Microbial Process for Food, Feeds, Energy, and Environment
Monday, Oct 30, 8:00 AM
MCC, 103B

Michael Tai, Chair
Joshua Yuan, Co-Chair
Ning Sun, Co-Chair

Sponsored by:
Innovations of Green Process Engineering for Sustainable Energy and Environment

8:00 Paper 95a: Coculture of Methanotrophs and Microalgae: A Flexible Platform for Biological CH_4/CO_2 Co-Utilization — ***Nathan Roberts***, *Min Hea Kim, Q. Peter He, Jin Wang*

8:20 Paper 95b: Identification of Antibiotic Resistome in Urban Watersheds via High-Throughput Screening
— *Adrian Low,* ***Jianzhong He***

8:40 Paper 95c: Influence of Subsurface Storage on the Microbiological and Physicochemical Quality of Surface Water
— ***Amit Kumar***, *Daphne H. P. Ng, Bin Cao*

9:00 Paper 95d: Use *Parageobacillus thermoglucosidasius:* Save the Planet
— ***Mohit Bibra***, *Aditi David, Glenn Johnson, Rajesh K. Sani*

9:20 Paper 95e: Efficient Preparation of β-O-4 Dilignols and Their Oxidative Coupling Studies
— ***Chang Peng***, *Zongbao Zhao*

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(96) Synthesis and Application of Porous Materials I: Synthesis and Characterization
Monday, Oct 30, 8:00 AM
MCC, 209A/B

Sunho Choi, Chair
Satish Nune, Co-Chair
Sandeep Kumar, Co-Chair

Sponsored by: Inorganic Materials

8:00 Paper 96a: Solution Combustion Synthesis of Porous CeO_2 Nanopowders: Reaction Mechanism and Physical Properties
— ***Wooram Kang***, *Derya Oncel Ozgur, Arvind Varma*

8:19 Paper 96b: Combining Pre- and Post-Nucleation Trajectories for the Design of Hierarchical FAU/EMT Materials from Organic-Free Sols
— ***Dina Gaber***, ***Safa Gaber***, *Issam Ismail, Saeed Alhassan,* ***Maryam Khaleel***

8:38 Paper 96c: Synthesis of Sn-MFI Zeolite with Use of Mechanochemical Reaction
— ***Kiyoshi Kanie***, *Moe Sakaguchi, Fumiya Muto, Masafumi Nakaya, Toshiyuki Yokoi, Atsushi Muramatsu*

8:57 Paper 96d: Crystallization of One-Dimensional Zeolites by Nonclassical Pathways
— ***Rui Li***, *James Sutjianto, Aseem Chawla, Jeffrey D. Rimer*

9:16 Paper 96e: Expanding the Scope of Fluoride-Free Pure Silica Zeolite Syntheses
— ***Vivek Vattipalli***, *Wei Fan*

9:35 Paper 96f: Atomic Resolution Imaging of MEL Intergrowth in 2-Dimensional MFI Nanosheets
— ***Prashant Kumar***, *Han Zhang, Neel Rangnekar, Michael Tsapatsis, K. Andre Mkhoyan*

9:54 Paper 96g: Synthesis of Single-Unit-Cell Hierarchical Zeolites with Tunable Mesoporosity by Controlling Intergrowth Frequency
— ***Dandan Xu***, *Anatoliy Kuznetsov, Prashant Kumar, Maryam Khaleel, Saeed Alhassan, Michael Tsapatsis*

10:13 Paper 96h: A Full Understanding of Microporous Vanadosilicate AM-6: The Crystal Quality and Structure of AM-6
— ***Rumeysa Tekin***, *Juliusz Warzywoda, Albert Sacco Jr.*

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(97) The Road Less Traveled: Professional Development for Teaching-Focused Faculty (Invited Talks)
Monday, Oct 30, 8:00 AM
MCC, 205C

Taryn Bayles, Co-Chair
Katie Cadwell, Co-Chair

Sponsored by:
Professional Development Committee Liaison

8:00 Paper 97a: Navigating the Unpaved Roads and Knowing the Unwritten Rules: Advancement for Teaching-Focused Faculty
— ***Lisa G. Bullard***

8:50 Break

9:00 Panel Discussion

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(98) Topical Plenary: Advanced Biomaterials, Biofuels, and Biorefinery (Invited Talks)
Monday, Oct 30, 8:00 AM
MCC, 200E

Yulin Deng, Chair
Shijie Liu, Co-Chair

Sponsored by:
Biorefinery Technologies for Forest-Based Lignocellulosic Biomass

8:00 Paper 98a: Rapid Wood Fractionation ≤ 80°C for Sustainable and Economic Biorefinery
— ***J. Y. Zhu***

8:25 Paper 98b: Insights into Biomass Recalcitrance
— ***Arthur J. Ragauskas***

8:50 Paper 98c: Low-Temperature and High-Efficiency Biomass Fuel Cell and Bio-Hydrogen Production
— ***Yulin Deng***

9:15 Paper 98d: Circular Economy: A Path Towards Innovation and Commercialization of Biocomposites for Sustainable Manufacturing
— ***Amar K. Mohanty***

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(99) Topical Plenary: Chemical Engineers in Medicine I (Invited Talks)
Monday, Oct 30, 8:00 AM
MCC, 202A/B

Swomitra Mohanty, Chair
Leonard F. Pease III, Co-Chair

Sponsored by:
Chemical Engineers in Medicine

8:00 Paper 99a: Overcoming Biological Barriers for Drug Delivery
— ***Samir Mitragotri***

8:40 Paper 99b: Engineering the Vocal Cords — ***Jennifer Long***

9:20 Paper 99c: Re-Engineering the Tumor Microenvironment to Enhance Efficacy of Molecular and Immune Therapies in Metastatic Cancer
— ***Paolo Provenzano***

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(100) World Café: Food-Energy-Water Nexus (Invited Talks)
Monday, Oct 30, 8:00 AM
MCC, 102A

JoAnn S. Lighty, Co-Chair
Hank Kohlbrand, Co-Chair

Sponsored by:
The Food-Energy-Water Nexus

8:00 Nexus Plenary and Topical Conference Overview

8:10 Paper 100a: Computing at the Nexus of Food, Energy, and Water
— ***Shashi Shekhar***

8:40 Paper 100b: Circling the Nexus
— ***Andrew Mangan***

9:10 Paper 100c: Limits to Growth and Global Sustainability of Food-Energy-Water Nexus — ***Urmila M. Diwekar,*** *Heriberto Cabezas*

9:40 Paper 100d: Improving Food Security within the Dynamics of the Food-Energy-Water Nexus
— ***Jack Starr***

10:10 Panel Discussion

10:25 Concluding Remarks

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(101) Student Design Competition
Monday, Oct 30, 8:30 AM
MCC, 103F

Sarah Ewing, Chair

Sponsored by:
Student Chapters Committee Liaison

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(102) Student Paper Competition
Monday, Oct 30, 8:30 AM
MCC, 103E

Keith M. Forward, Chair

Sponsored by:
Student Chapters Committee Liaison

8:30 Paper 102a: A Fiberless Adenovirus Vector for Delivering the GFP Reporter Gene
— ***Anna Condacse***

8:50 Paper 102b: Protein Nanocarrier for Targeted Intracellular Delivery of Functional Antibodies
— ***Cyril Lukianov***, *Sung In Lim, Julie A. Champion*

9:10 Paper 102c: Novel Chemistries and Engineering for the Replacement of Methylenedianiline in Composites
— ***Jayson D. Cosgrove***, *Kevin M. Schmalbach, Owen M. Stecca, Alexander W. Bassett, William S. Eck, Craig M. Paquette, Joshua Sadler, John La Scala, Joseph F. Stanzione III*

9:30 Paper 102d: Free Surface Electrospinning of Microemulsions Containing Fenofibrate
— ***Katarina Guzman***, *Thai Nguyen, Uyen Phan, Jack Lift, Hovhannes Gregorchuk, Keith M. Forward*

9:50 Paper 102e: Polyvinyl Sulfonic Acid: A Low-Cost RNase Inhibitor for Enhanced RNA Preservation and Retained Function
— ***Conner C. Earl***, *Mark T. Smith, Richard A. Lease, Bradley C. Bundy*

10:10 Paper 102f: A Stimulus-Responsive, In-Situ-Forming, Nanoparticle-Laden Hydrogel for Ocular Drug Delivery
— ***Syed H. Kamal***, *Maryam Kabiri, Sandip V. Pawar, Sazzad Hossain, Vikramaditya Yadav*

10:30 Paper 102g: Single-Use, In-Vitro Biosensors for the Detection of T-Tau Protein and Beta-Amyloid 42, Biomarkers of Neuro-Degenerative Disorders in PBS & Human Serum Using Differential Pulse Voltammetry (DPV) — ***Yifan Dai***, *Chung-Chiun Liu*

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(103) Electrokinetics for Cellular Analysis & Separation
Monday, Oct 30, 9:00 AM
Hilton, Marquette IV/V/VI/VII

Hadi Shafiee, Chair
Ezekiel Adekanmbi, Co-Chair

Sponsored by:
2017 Annual Meeting of the AES Electrophoresis Society

9:00 Paper 103a: Organelle Separation with a Microfluidic Ratchet
— ***Alexandra Ros***, *Edgar A. Arriaga, Daihyun Kim*

9:15 Paper 103b: Cell Surface Complexity Modulates Membrane Capacitance and Differentiation of Human Neural Stem Cells
— ***Shubha Tiwari***, *Estelle Kim, Jamison Nourse, Citra Soemardy, Lisa A. Flanagan*

9:30 Paper 103c: Characterizing Human Embryonic Stem Cells Function with Dielectrophoresis and Flow Cytometry — ***Tayloria N. G. Adams***, *Clarissa C. Ro, Shubha Tiwari, Lisa A. Flanagan*

9:45 Paper 103d: Electrical Detection of Zika Virus on Paper Microchip with Silver-Graphene-Nano-Composite Electrode — *Mohamed Draz, Harini Lakshminarayanan, Manasa Venkataramani, Kamyar Mehrabi, Maryam Moazeni,* ***Hadi Shafiee***

10:00 Paper 103e: Characterization of Dielectrophoretic Response of *Candida* Cells Using 3D Carbon-Electrode Dielectrophoresis
— *Monsur Islam,* ***Jordon Gilmore***, *Rodrigo Martinez-Duarte*

10:15 Paper 103f: A Method for the Sustainable Synthesis of Carbon Fibers Using Dielectrophoresis of Bacteria and Pyrolysis — ***Devin Keck***, *Monsur Islam, Rodrigo Martinez-Duarte*

10:30 Paper 103g: Microscale Extraction of Rare Earth Elements Using Biosorption and Dielectrophoresis
— ***Ezekiel Adekanmbi***, *Soumya Srivastava*

10:45 Paper 103h: Electrophysiology of *Borrelia burgdorferi*
— ***Ezekiel Adekanmbi***, *Soumya Srivastava*

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(104) Networking for Nerds: How to Land (or Create) Your Dream Job and Keep Your Career Moving Forward! (Invited Talks)
Monday, Oct 30, 9:30 AM
MCC, 101A

April Grasso, Chair
Steve Smith, Co-Chair

Sponsored by: Publication Committee

9:30 Paper 104a: Networking for Nerds: How to Land (or Create) Your Dream Job and Keep Your Career Moving Forward! — ***Alaina Levine***

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(105) Undergraduate Student Poster Session: Catalysis and Reaction Engineering
Monday, Oct 30, 10:00 AM
MCC, Exhibit Hall B

Victor Breedveld, Chair

Sponsored by:
Student Chapters Committee Liaison

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(106) Undergraduate Student Poster Session: Computing and Process Control
Monday, Oct 30, 10:00 AM
MCC, Exhibit Hall B

Victor Breedveld, Chair

Sponsored by:
Student Chapters Committee Liaison

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(107) Undergraduate Student Poster Session: Education & General Papers
Monday, Oct 30, 10:00 AM
MCC, Exhibit Hall B

Victor Breedveld, Chair

Sponsored by:
Student Chapters Committee Liaison

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(108) Undergraduate Student Poster Session: Environmental
Monday, Oct 30, 10:00 AM
MCC, Exhibit Hall B

Victor Breedveld, Chair

Sponsored by:
Student Chapters Committee Liaison

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(109) Undergraduate Student Poster Session: Food, Pharmaceutical, and Biotechnology
Monday, Oct 30, 10:00 AM
MCC, Exhibit Hall B

Victor Breedveld, Chair

Sponsored by:
Student Chapters Committee Liaison

(110) Undergraduate Student Poster Session: Fuels, Petrochemicals, and Energy
Monday, Oct 30, 10:00 AM
MCC, Exhibit Hall B

Victor Breedveld, Chair

Sponsored by:
Student Chapters Committee Liaison

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(111) Undergraduate Student Poster Session: Materials Engineering and Sciences
Monday, Oct 30, 10:00 AM
MCC, Exhibit Hall B

Victor Breedveld, Chair

Sponsored by:
Student Chapters Committee Liaison

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(112) Undergraduate Student Poster Session: Separations
Monday, Oct 30, 10:00 AM
MCC, Exhibit Hall B

Victor Breedveld, Chair

Sponsored by:
Student Chapters Committee Liaison

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(113) Undergraduate Student Poster Session: Sustainability
Monday, Oct 30, 10:00 AM
MCC, Exhibit Hall B

Victor Breedveld, Chair

Sponsored by:
Student Chapters Committee Liaison

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(114) Meet the Executives: Innovating for a Sustainable Future (Invited Talks)
Monday, Oct 30, 11:00 AM
MCC, Ballroom B

Sipho C. Ndlela, Chair
David Reeder, Co-Chair

Sponsored by: Miscellaneous

11:00 Introductory Remarks

11:10 Paper 114a: Sustaining Innovation / Innovating Sustainably
— ***A. N. Sreeram***

11:25 Paper 114b: Presentation by Panelist — ***Chris Mallett***

11:40 Paper 114c: Innovating for a Sustainable Future — ***Teressa Szelest***

11:55 Paper 114d: Owens Corning: Continued Delivery on Impactful Sustainable and Innovative Business and R&D Strategies
— ***Jose Luis Mendez-Andino***

12:10 Paper 114e: Panel Discussion
— ***S. Shariq Yosufzai***

(115) WIC Luncheon (Ticketed Event)
Monday, Oct 30, 11:00 AM
Hilton, Minneapolis Ballroom C

Heather N. Emady, Chair
Julianne L. Holloway, Co-Chair

Sponsored by:
Women's Initiatives Committee

11:00 AM Paper 115a: Planning, Serendipity, and Optimism: Key Components of a Career in Progress
— ***Rachel Segalman***

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(116) Poster Presentation Success: How to Prepare and Present a Winning Poster (Invited Talks)
Monday, Oct 30, 12:30 PM
MCC, 101A

April Grasso, Chair
Steve Smith, Co-Chair

Sponsored by:
Publication Committee

12:30 Paper 116a: Poster Presentation Success — ***Alaina Levine***

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(117) Using Trade Secrets to Protect Chemical Process Innovations
Monday, Oct 30, 12:30 PM
MCC, M100F

Sponsored by:
Chemical Engineering & the Law Forum

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(118) Advanced Structural Composites
Friday, Nov 3, 8:00 AM
MCC, 102C

Jiahua Zhu, Chair
Shuangliang Zhao Sr., Co-Chair
Kenan Song, Co-Chair
Pingwei Liu, Co-Chair

Sponsored by: Composites

8:00 Paper 118a: Improvement of Thermal Conductivity for POSS-Functionalized BN Fillers/Polyphenylene Sulfide Composites
— ***Xutong Yang***, *Lin Tang, Yongqiang Guo, Junwei Gu*

8:15 Paper 118i: Structural Composites with Multiple Functionalities — ***Kenan Song***

8:30 Paper 118c: Fabrication of High-Dispersed Strawberry-Like P (St-*co*-MAA)/SiO_2 Composite Microspheres and Their Applications in Mortar — ***Guanzhi Cheng,***
Huajian Li, Xinguo Zheng, Yongjian Xie, Jing Liu

8:45 Paper 118d: Hydrogen-Bonded Thermal Highways Driving Heat Conduction in Polymer and Polymer Blends Films
— ***Nitin Mehra***, *Jiahua Zhu*

9:00 Paper 118e: Low-Temperature Synthesis of Mn-Based Mixed Metal Oxides with Novel Fluffy Structures as Efficient Catalysts for FTO Reaction
— ***Yi-Fan Han***, *Bo Meng*

9:15 Paper 118f: Structural Control of Polybenzoxazine/Epoxy Composites with Dual Crosslinking Network for Corrosion Protection
— ***Changlu Zhou***, *Zhong Xin*

9:30 Paper 118g: Multifunctional Epoxy Conductive Nanocomposites
— ***Xiaojiang Xu***, *Hongbo Gu*

9:45 Paper 118h: Nano-Structured Ceramic ALD Coatings to Stabilize SiC Against Reaction in High-Temperature Steam
— ***Amanda Hoskins***, *Aidan Coffey, Charles B. Musgrave, Alan W. Weimer*

10:00 Paper 118j: Multi-Scale Metrology for Visualization and Characterization of Interphase Failure
— ***Richard Sheridan***,
Jeremiah Woodcock, Jeffrey W. Gilman, Gale Holmes, Catherine Brinson, Vamshi Gudapati, Dave Hartman, Amol Vaidya

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(119) Advances in Metabolic Engineering of Photosynthetic/ Non-Model Organisms
Monday, Oct 30, 12:30 PM
MCC, 206A/B

Kevin V. Solomon, Chair
Zengyi Shao, Co-Chair

Sponsored by: Bioengineering

12:30 Break

12:48 Paper 119b: Modeling-Guided Engineering Enables Efficient Limonene Production in Cyanobacteria — *Xin Wang,* ***Joshua Yuan***

1:06 Paper 119c: Engineering an Environmentally Isolated Strain of *Bacillus megaterium* for Biofuel Production and Recovery Under Supercritical CO_2
— ***Jason T. Boock***,
Adam J. E. Freedman, Geoffrey Tompsett, Michael T. Timko, Janelle R. Thompson, Kristala L. J. Prather

1:24 Paper 119d: Development and Application of a CRISPRi System for the Syngas-Fermenting Microbe *Clostridium ljungdahlii*
— ***Benjamin Woolston***,
David Emerson, Devin Currie, Gregory Stephanopoulos

1:42 Paper 119e: Cyanobacterial Glycogen Production and Hydrolysis for Production of Media for Industrial Bioprocessing
— ***Austin D. Comer,***
Wenzhao (Tony) Wu, Christos T. Maravelias, Brian Pfleger

2:00 Paper 119f: Deciphering Cyanobacterial Phenotypes for Fast Photoautotrophic Growth
— ***Mary Abernathy***, *Jingjie Yu, Fangfang Ma, Michelle Liberton, Justin Ungerer, Whitney D. Hollinshead, Saratram Gopalakrishnan, Lian He, Costas D. Maranas, Himadri B. Pakrasi, Douglas K. Allen, Yinjie Tang*

2:18 Paper 119g: Metabolite Cross-Feeding Drives the Symbiotic Growth of *Chlorella vulgaris* and Heterotrophic Microbes — ***Maciek Antoniewicz***

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(120) Advances in Optimization I
Monday, Oct 30, 12:30 PM
MCC, 103E

Joseph Scott, Chair
Ruth Misener, Co-Chair

Sponsored by:
Computers in Operations and Information Processing

12:30 Paper 120a: Bilevel Programs with Coupling Equality Constraints for Parameter Estimation of Thermodynamic Property Models
— *Hatim Djelassi, Moll Glass,* ***Alexander Mitsos***

12:51 Paper 120b: A Branch and Bound Algorithm to Solve Large-Scale Multistage Stochastic Programs
— ***Brianna Christian***,
Selen Cremaschi

1:12 Paper 120c: A New Decomposition Framework for Solving Multi-Stage Stochastic Programs with Endogenous Uncertainty
— ***Zuo Zeng***, *Brianna Christian, Selen Cremaschi*

1:33 Paper 120d: A Framework for Modeling and Optimizing Complex, Structured Problems
— ***Bethany Nicholson***, *John D. Siirola*

1:54 Paper 120e: Identification of Optimization Decomposition Structures via Community Detection Algorithms
— ***Andrew Allman***, *Wentao Tang, Prodromos Daoutidis*

2:15 Paper 120f: Integrating Mixed-Integer Optimisation and Satisfiability Modulo Theories — *Miten Mistry,* ***Ruth Misener***

2:36 Paper 120g: Solution Methods for Multiperiod Blend Scheduling MINLP Models — ***Yifu Chen***,
Christos T. Maravelias

(121) Applied Environmental Catalysis I
Monday, Oct 30, 12:30 PM
MCC, L100B

Di Wang, Chair
Eleni A. Kyriakidou, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

12:30 Paper 121a: Experimental Study of Hydrocarbon Trapping over Passive NO_x Adsorber — ***Sam Malamis***

12:48 Paper 121b: CuO/Co_3O_4: A Highly Active and Selective Low-Temperature NO Decomposition Catalyst
— ***Torin C. Peck***,
Krishna Reddy Gunugunuri, Charles A. Roberts

1:06 Paper 121c: Effect of Different Structure-Directing Agents on Deactivation of Cu/SAPO-34 During Low-Temperature NH_3-SCR
— ***Jungwon Woo***, *Kirsten Leistner, Mark Shost, Holmes Ahari, Mike Zammit, Louise Olsson*

1:24 Paper 121d: A Perovskite-Like Catalyst for the Simultaneous Removal of Soot and NO: Effect of the Synthesis Method
— ***Laura Urán***, *Jaime Gallego, Alexander Santamaria*

1:42 Paper 121e: Fast Cycling to Achieve High-NO_x Conversion in Lean Exhaust: Role of Ceria
— ***Zhiyu Zhou***, *Michael Harold, Dan Luss*

2:00 Paper 121f: NO Reduction by CO over CeO_2 Supported Co_xO_y Catalysts
— ***Shuhao Zhang***, *Nusnin Akter, Da Qu, Jinyue Pan, Taejin Kim, Yuanyuan Li, Jiahao Huang, Anatoly I. Frenkel*

2:18 Paper 121g: Nb_2O_5-Promoted Base Metal Oxide Catalysts Used for Air Pollution Abatement in Stationary Plants
— ***Sogand Aghamohammadi***, *Wendi Xiang, Robert Farrauto*

2:36 Paper 121h: N-Doped TiO_2 Nanoparticles Synthesized by One-Step Liquid Flame Aerosol Method (LFSP): Understanding the Effect of Synthesis Parameters and Photocatalytic Degradation of VOCs
— *Panagiotis Smirniotis,* ***Siva Nagi Reddy Inturi***, *Makram Suidan*

(122) Area Plenary: Adsorption and Ion Exchange I — In Honor of Douglas M. Ruthven (Invited Talks)
Monday, Oct 30, 12:30 PM
MCC, M100E

Matthias Thommes, Chair
Stefano Brandani, Co-Chair

Sponsored by:
Adsorption and Ion Exchange

12:30 Introductory Remarks

12:35 Paper 122a: Diffusion in Nanopores Under the Microscope
— ***Jörg Kärger***, *Tomas Binder, Juergen Caro, Christian Chmelik, Dieter Freude, Juergen Haase, Lars Heinke, Alexander Lauerer, Rustem Valiullin*

1:00 Paper 122b: Transport in Small-Pore Zeolites — ***Peter I. Ravikovitch***, *Harry W. Deckman*

1:20 Paper 122c: Process-Based Adsorbent Screening and Design for Post-Combustion CO_2 Capture by Vacuum Swing Adsorption
— ***Arvind Rajendran,***
Shamsuzzaman Farooq

1:40 Paper 122d: Using a Volumetric Apparatus to Distinguish Between Diffusion and Surface-Resistance Mass-Transfer Kinetics in Commercial Adsorbents — ***Federico Brandani***, *Pluton Pullumbi, Stefano Brandani*

2:00 Paper 122e: Development of Sour PSA Technology for Gasification Markets — ***Jeffrey R. Hufton***

2:20 Paper 122f: Separations Inspired from Adsorption: From Adsorbents to Adsorbent Membranes
— ***F. Handan Tezel***

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(123) Area Plenary: Emerging Areas in Polymer Science and Engineering II — Area 8A (Invited Talks)
Monday, Oct 30, 12:30 PM
MCC, 211B

Santanu Kundu, Chair
Ying Diao, Co-Chair

Sponsored by: Polymers

12:30 Paper 123a: Active Polymer Materials for Flexible Electronics: Molecular Design and Processing for Efficient Macroscale Charge Transport Pathways
— *Nils Persson, Michael McBride, Ping-Hsun Chu, Martha A. Grover,* ***Elsa Reichmanis***

1:05 Paper 123b: Promoting Adhesion Between Immiscible Polymers
— ***Christopher W. Macosko***

1:40 Paper 123c: High-Resolution Lithography via Block Copolymers and Self-Assembling Surface Neutral Layers — ***Peter Trefonas III***, *Jong Keun Park, Mingqi Li, Janet Wu, Emad Aqad, Dan Millward, Valeriy Ginzburg, Phil Hustad*

2:15 Paper 123d: Field- and Confinement-Directed Self-Assembly of Soft Mesophases to Create Useful Materials — ***Chinedum O. Osuji***

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(124) Area Plenary: Crystallization and Evaporation — Area 2B (Invited Talks)
Monday, Oct 30, 12:30 PM
MCC, M100J

Marina Tsianou, Chair
Seth Huggins, Co-Chair

Sponsored by:
Crystallization and Evaporation

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(125) Area Plenary: Future Directions in Applied Mathematics and Numerical Analysis (Invited Talks)
Monday, Oct 30, 12:30 PM
MCC, 103F

Martin Guay, Chair
Ashlee N. Ford Versypt, Co-Chair

Sponsored by:
Applied Mathematics and Numerical Analysis

12:30 Paper 125a: Servo-Control of Selective Catalytic Reduction in Diesel-Powered Vehicles
— ***Xiaodong Xu***, *Stevan Dubljevic*

12:55 Paper 125b: A Parallel Fluid-Solid Coupling Model with Lattice Boltzmann Fluid Solver and Molecular Dynamics Simulator Using the Immersed Boundary Method
— ***Jifu Tan***, *Talid Sinno, Scott L. Diamond*

1:20 Paper 125c: Efficient Linear Underestimators for Dynamic Process Systems — ***Kamil A. Khan***

1:45 Paper 125d: Model Misspecifications in Metabolic Flux Analysis: Biases, Tests and Fixes
— ***Rudiyanto Gunawan***,
Sandro Hutter

2:10 Paper 125e: Optimal Flow Control for Oil Production Under Gas Coning Conditions in Oil-Rim Reservoirs
— ***Prashanth Siddhamshetty***,
Joseph Sangil Kwon

(126) Area Plenary: Leaders in Biomaterials (Invited Talks)
Monday, Oct 30, 12:30 PM
MCC, 211C

Jorge Almodovar, Chair
Shannon L. Servoss, Co-Chair
Eun Ji Chung, Co-Chair

Sponsored by: Biomaterials

12:30 Paper 126a: Nanostructured Interfaces for Enhanced Biologic Transport and Immunomodulation
— ***Tejal Desai***

1:15 Paper 126b: Nano- and Microfabricated Hydrogels for Regenerative Engineering
— ***Ali Khademhosseini***

2:00 Paper 126c: Overcoming Obstacles to Brain Repair Using Biomaterials — ***Tatiana Segura***

2:45 Panel Discussion

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(127) Atomically Dispersed Supported Metal Catalysts II
Monday, Oct 30, 12:30 PM
MCC, L100F

Jean-Sabin McEwen, Chair
Ning Yan, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

12:30 Paper 127a: CO_2 Reduction over Metal-Cluster/TiO_2 Photocatalysts
— ***Satish Iyemperumal***,
N. Aaron Deskins

12:50 Paper 127b: Unsupported and Supported Au_1-O_x-$(OH)_y$-Na_z Clusters as Stable, Single-Site Gold Catalysts
— ***Sufeng Cao***, *Ming Yang, Chongyang Wang, Ahmed Elnabawy, Jilei Liu, Antonios Trimpalis, Junjun Shan, Sungsik Lee, Mengwei Li, Lawrence Allard, Manos Mavrikakis, Maria Flytzani-Stephanopoulos*

1:10 Paper 127c: Atomically Dispersed Rhodium on Self-Assembled Phosphotungstic Acid: Structural Features and Catalytic CO Oxidation Properties — *Bin Zhang, Ning Yan*

1:30 Paper 127d: High-CO Oxidation Activity on Pt Single Atoms and Clusters Supported on $MgAl_2O_4$
— ***Chun-Te Kuo***, *Yubing Lu, Xiwen Zhang, Ayman M. Karim*

1:50 Paper 127e: Transition Metal–Doped Graphene for the CO_2 Reduction Reaction — ***Leanne Chen***,
Thomas Miller III

2:10 Paper 127f: Ni/Cerium-Titanium Oxide Catalyst for Dry Reforming of Methane — ***Sachin Nandanwar***,
Yunkai Zou, Joseph Holles, Jing Zhou, Samantha Hulett, Michael Cuddy

2:30 Paper 127g: Tuning the Interfacial Property of Copper-Ceria Catalyst by Indium for Low-Temperature CO Oxidation — ***Xiao-man Zhang***, *Jing Xu, Yifan Han*

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(128) Biochemical & Biotechnology U.G. Research Session (Invited Talks)
Monday, Oct 30, 12:30 PM
MCC, 101H

Colin Young, Chair
Rose Damestani, Co-Chair

Sponsored by:
Young Professionals Committee (YPC)

12:30 Paper 128a: Densification of Biomass By Using Natural and Synthetic Binder — ***Tabish Ali Zeb***

12:55 Paper 128b: Next Generation Oxygen Recovery for Exploration Life Support — ***Sarah Kelly***

1:20 Paper 128c: Antibody Adsorption on Fluid-Fluid Interface — ***Mariia Chernova***

1:45 Paper 128d: Liposome Production and Concomitant Loading of Drug Simulants By Microfluidic Hydrodynamic Focusing — ***Wan-Zhen Lin***, *Noah Malmstadt*

2:10 Paper 128e: Tuning Size and Charge of a Multivalent Polymer Library for Enhanced Drug Delivery to Cartilage — ***Salwan Butrus***

2:35 Paper 128f: Building Brains: Marrying Engineering & Medicine in the Fight Against Alzheimer Disease — ***Athanasios Kritharis***

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(129) Biochemical Conversion Processes in Forest/Plant Biomass Biorefineries
Monday, Oct 30, 12:30 PM
MCC, 200E

Shijie Liu, Chair
Zhiliang (Julia) Fan, Co-Chair

Sponsored by:
Biorefinery Technologies for Forest-Based Lignocellulosic Biomass

12:30 Paper 129a: Bridging the Gap Between Feedstock Growers and Users: A Study of Poplar Coppice-Based Biorefinery — *Rick Gustafson*, ***Chang Dou, Renata Bura***

12:51 Paper 129b: Study on Liquefaction of Straw Biomass Catalyzed by Sulfonate Ionic Liquid [HSO_3-BMIM][HSO_4] in Ethanol — ***Qian Guan***, *Tingzhou Lei, Zhiwei Wang, Haiyan Xu, Gaofeng Chen, Xueqin Li, Zijie Li*

1:12 Paper 129c Douglas Fir Tannin Inhibition of *Trichoderma reesei* Cellulase — ***Karl Oleson***, *Kayla Sprenger, Jim Pfaendtner, Daniel T. Schwartz*

1:33 Paper 129d: Process Kinetics of Mixed Bacteria Photosynthetic Hydrogen Production — ***Yanyan Jing***, *Chao He, Yi Wang*

1:54 Paper 129e: Inhibition Effect of Aromatic Aldehydes on Butanol Fermentation by *Clostridium acetobutylicum* — *Jing Li*, ***Maobing Tu***

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(130) Biosensor Devices: Applications
Monday, Oct 30, 12:30 PM
MCC, M100A

Jeffrey M. Halpern, Chair
Evan K. Wujcik, Co-Chair
Ryan Hansen, Co-Chair

Sponsored by: Sensors

12:30 Paper 130h: The Development of a Sensitive Electrochemical Method for Carotenoid Detection — ***Sabrina Marnoto,*** *Jeffrey M. Halpern*

12:45 Paper 130b: A Radio-Colorimetric Hydrogel for Detection of Therapeutic Levels of Ionizing Radiation Using Plasmonic Nanoparticles in 3D — ***Karthik Pushpavanam***, *Sahil Inamdar, Tomasz Bista, Stephen Sapareto, Kaushal Rege*

1:00 Paper 130d: Thermodynamic Control of Response in Ionophore-Based Optical Nanosensors — ***Mark S. Ferris,*** *Aakash G. Katageri, Makayla K. Elms, Greta M. Gohring, Kevin J. Cash*

1:30 Paper 130e: Combining Forward Osmosis with Electrochemistry to Detect Ultra-Low Concentrations of Bacterial Virulence Factors and Quorum-Sensing Molecules in Bodily Fluids — ***Martin K. Kimani***, *Hunter J. Sismaet, Edgar D. Goluch*

1:45 Paper 130f: Healthcare Technology Platforms: Engineering a Cellulose Strip for Biomarker Detection — *Akshay Subramaniam,* ***Ramchander Chepyala***, *Serena Stephen D. Souza, Santosh B. Noronha*

2:00 Paper 130g: A Novel Modified DOT Blot Approach for Early Detection of Osteoporosis on Cellulose Substrates — ***Serena Stephen D. Souza***, *Ramchander Chepyala, Santosh B. Noronha*

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(131) Carbon Nanomaterials Graduate Student Award Session
Monday, Oct 30, 12:30 PM
MCC, 213A/B

Anson Ma, Chair
Micah Green, Co-Chair
Anju Gupta, Co-Chair

Sponsored by: Carbon Nanomaterials

12:30 Paper 131a: Ionophore-Decorated Phosphazene-Functionalized Magnetic Graphene Oxide as a Composite Adsorbent Material for Selective Lithium-Ion Recovery — ***Khino J. Parohinog***, *Grace M. Nisola, Wook-Jin Chung*

12:45 Paper 131b: Ion Transport Through Carbon Nanotubes: A Molecular Dynamics Study — ***Michelle Aranha***, *Brian J. Edwards*

1:00 Paper 131d: Antibody-Mimetic Protein Detection with Peptoid-Functionalized Near-Infrared Carbon Nanotube Optical Sensors — ***Linda Chio***, *Jackson Travis Del Bonis-O'Donnell, Mark Kline, Ronald N. Zuckermann, Markita Landry*

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(132) Catalytic Processing of Fossil and Biorenewable Feedstocks II: Carboxylic Acids and Ketones
Monday, Oct 30, 12:30 PM
MCC, L100C

Zhenglong Li, Chair
Steven Crossley, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

12:30 Paper 132a: Renewable Isoprene by Sequential Hydrogenation of Itaconic Acid and Dehydra-Decyclization of 3-Methyl-Tetrahydrofuran — ***Omar A. Abdelrahman***, *Dae Sung Park, Katherine P. Vinter, Charles S. Spanjers, Limin Ren, Hong Je Cho, Kechun Zhang, Wei Fan, Michael Tsapatsis, Paul J. Dauenhauer*

12:50 Paper 132b: Using Microkinetic Analysis to Predict Product Selectivity During Propionic Acid Hydrodeoxygenation over Supported Pt and Ru Catalysis — ***Joshua Gopeesingh,*** *Jesse Q. Bond*

1:10 Paper 132c: Renewable Adipic Acid Production via Metal-Free Cleavage of C-O Bonds in the Presence of Molecular H_2 in Organic Acid Solvents — *Matthew Gilkey, Alexander V. Mironenko, Dion Vlachos,* ***Bingjun Xu***

1:30 Paper 132d: Influence of Sn Promoter on Pd and Pt Catalysts for Conversion of Heptanoic Acid and Propane — ***Nicholas Kaylor***, *Jiahan Xie, Yong-Su Kim, Hien N. Pham, Abhaya K. Datye, Yong-Kul Lee, Robert J. Davis*

1:50 Paper 132e: Selectivity Control During the One-Pot Conversion of Aliphatic Carboxylic Acids to Linear Olefins Through Tandem Hydrogenation/Dehydration — ***Jher Hau Yeap***, *Bartosz Rozmysłowicz, Jeremy S. Luterbacher*

2:10 Paper 132f: Catalyst for Conversion of Methyl Ethyl Ketone to Butenes — ***Zahraa Alauda***, *Hayder Alatabi, Quanxing Zheng, Keith Hohn*

2:30 Paper 132g: Conversion of C6 Sugars to Alpha-Hydroxy Acids over Lewis Acidic Hf-, Sn-, and Zr- Beta Zeolite Catalysts Using γ-Valerolactone as Solvent — ***Isabel Hortal-Sánchez***, *Christian G. Rivera-Goyco, Yomaira J. Pagan-Torres, Nelson Cardona-Martínez*

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(133) Chemical Conversion Processes in Forest/Plant Biorefineries
Monday, Oct 30, 12:30 PM
MCC, 200D

Bin Liang, Chair
Sasidhar Varanasi, Co-Chair

Sponsored by:
Biorefinery Technologies for Forest-Based Lignocellulosic Biomass

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(134) Chemical Engineering Principles Advancing Medicine I
Monday, Oct 30, 12:30 PM
MCC, 202A/B

Charles Reid, Chair
Thomas A. Zangle, Co-Chair

Sponsored by:
Chemical Engineers in Medicine

12:30 Paper 134a: Heat Transfer Effects on *Staphylococcus epidermidis* Biofilms: An In-Vitro Catheter Model — ***Joanne Beckwith***, *J. Scott Van Epps, Michael J. Solomon, Usha Kadiyala*

12:52 Paper 134b: Elucidating the Physiological Significance of Nitric Oxide Synthase (NOS) in *Staphylococcus aureus* Through Metabolic Modeling — ***Mohammad Mazharul Islam***, *Rajib Saha, Sujata Chaudhari, Vinai Chittezham Thomas*

1:14 Paper 134c: Regulating Fibrin Formation, Structure, and Mechanical Strength — *Joanna L. Sylman, Uranbileg Daalkhaijav,* ***Travis W. Walker***, *Owen J. T. McCarty*

1:36 Paper 134d: Roles of Conserved Tryptophans in Trimerization of HIV-1 Membrane-Proximal External Regions: Implications for Virucidal Design via Alchemical Free-Energy Molecular Simulations — ***Steven T. Gossert,*** *Bibek Parajuli, Irwin Chaiken, Cameron F. Abrams*

1:58 Paper 134e: Mathematical Modeling of Ultrasound in Regenerative Medicine: From the Cellular Scale to the Macroscale — ***Anu Subramanian***, *Hendrik Viljoen, April Miller*

2:20 Paper 134f: Kelvin–Helmholtz Instabilities During Bacterial Separation from Blood — ***Ryan Wood***, *Daniel Mc Clellan, Jared Whitehead, William G. Pitt*

2:42 Paper 134g: Dynamic Deformation of the Cell Plastically Shapes the Nucleus and Amplifies Cancer Nuclear Irregularities — ***Vincent J. Tocco Jr.***, *Yuan Li, Richard Dickinson, Tanmay Lele*

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(135) Chemical-Looping Processes I
Monday, Oct 30, 12:30 PM
MCC, 103A

Kevin Whitty, Chair
JoAnn S. Lighty, Co-Chair
Shwetha Ramkumar, Co-Chair
Samuel Bayham, Co-Chair

Sponsored by:
Innovations of Green Process Engineering for Sustainable Energy and Environment

12:30 Paper 135a: Development of Unique Trimetallic Copper-Iron-Manganese Oxygen Carrier for Chemical-Looping Combustion — ***William Benincosa III***, *Ranjani V. Siriwardane, Hanjing Tian, Jarrett Riley*

12:51 Paper 135b: Dopant-Modified Iron-Based Materials for Fuel Chemical-Looping Combustion and Reforming Applications — ***Mengqing Guo***, *Lang Qin, Zhuo Cheng, Yan Liu, Dikai Xu, Jonathan A. Fan, Liang-Shih Fan*

1:13 Paper 135c: Tuning Bulk and Surface Properties of Mixed Metal Oxides for Partial Oxidation Applications via Chemical-Looping Schemes — ***Fanxing Li***

1:34 Paper 135d: Microstructure and Mechanical Strength Evolution of Iron Oxide in Chemical-Looping Combustion — ***Zhong Ma***, *Rui Xiao*

1:56 Paper 135e: Continuous Large-Scale Production of Red Mud Oxygen Carriers with a Rotary Kiln for Chemical-Looping Combustion — ***Jinhua Bao***, *Liang Kong, Zhen Fan, Heather Nikolic, Kunlei Liu*

2:17 Paper 135f: Correlation of the Physical and Solid-State Chemistry Changes for a CuO-Fe_2O_3-Al_2O_3 Oxygen Carrier During Reduction with H_2 and CO for Chemical-Looping Combustion Applications — ***Jarrett Riley***, *Ranjani V. Siriwardane, Hanjing Tian, William Benincosa III*

2:39 Paper 135g: Chemical-Looping Partial Oxidation of Solid Fuels for High-Purity Syngas Production — ***Tien-Lin Hsieh***, *Dikai Xu, Yitao Zhang, Mengqing Guo, Dawei Wang, Cheng Chung, Zhuo Cheng, Lang Qin, Pengfei He, Mingyuan Xu, Yaswanth Pottimurthy, Yu-Yen Chen, Cody Park, Liang-Shih Fan, Andrew Tong*

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(136) Computational Solid-State Pharmaceutics
Monday, Oct 30, 12:30 PM
MCC, 204A/B

Yuriy Abramov, Chair
Susan M. Reutzel-Edens, Co-Chair

Sponsored by:
Pharmaceutical Discovery, Development and Manufacturing Forum

12:30 Paper 136a: Accurate and Efficient Representation of Intramolecular Energy in Ab-Initio Generation of Crystal Structures — ***Isaac Sugden***, *Claire S. Adjiman, Costas C. Pantelides, Christina-Anna Gatsiou*

12:51 Paper 136b: A New Approach in Applying CSP for the Pharmaceutical Industry — ***Alan Jiang***, *Shuhao Wen*

1:12 Paper 136c: Capturing the Role of Temperature and the Sensitivity to Energy Function Complexity in Crystal Polymorph Stability Using Molecular Modeling — *Eric Dybeck, Nathan Abraham, Natalie Schieber,* ***Michael R. Shirts***

1:33 Paper 136d: Can Lattice Dynamics with Anisotropic and Isotropic Thermal Expansion Accurately Estimate Thermodynamic Properties of Crystals Pharmaceutics Compared to Molecular Dynamics? — ***Nathan Abraham***, *Eric Dybeck, Natalie Schieber, Michael Shirts*

1:54 Paper 136e: Prediction of Phase Transition Thermodynamics for Crystals of Pharmaceutical Compounds — ***Olexandr Isayev***, *Alexander Golbraikh, Eugene Muratov, Yuriy Abramov, Alexander Tropsha*

2:15 Paper 136f: Crystal Engineering Applications of COSMO-RS — *Christoph Loschen,* ***Jens Reinisch***, *Andreas Klamt*

2:36 Paper 136g: Enabling Rational Morphology Design and Crystal Engineering with Addict Software for Mechanistic Crystal Growth Models — ***Peng Zhu***, *Jinjin Li, Carl Tilbury, Yuanyuan Sun, Kevin Girard, Yuriy Abramov, Michael F. Doherty*

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(137) Control and Optimization of Particle and Solids Production
Monday, Oct 30, 12:30 PM
MCC, 200H

Heather N. Emady, Chair
Bryan J. Ennis, Co-Chair

Sponsored by:
Particle Production and Characterization

12:30 Paper 137a: Quantitative Validation and Analysis of Heat Transfer in a Rotary Drum Using Experiments and Simulations — ***Manogna Adepu***

12:50 Paper 137b: A Comparison of Numerical Optimization Methods for Cyclone Separators — ***Rafaello Duarte Luciano,*** *Leonardo Machado da Rosa, Henry F. Meier*

1:10 Paper 137c: Optimization of Cyclone Separators in Series Based on Computational Fluid Dynamics — ***Rafaello Duarte Luciano***, *Leonardo Machado da Rosa, Henry F. Meier*

1:30 Paper 137d: Application of Psychrometric Principles for Predicting the Bulk Density of Spray-Dried Dispersions — ***Ariel R. Muliadi***, *Joseph W. Bullard*

1:50 Paper 137e: A Model-Guided Selection of Media Size in Wet Stirred Media Milling of Poorly Water-Soluble Drugs — ***Ecevit Bilgili***, *Paulina Alvarez, Meng Li*

2:10 Paper 137f: Reduced-Order Discrete Element Method Modeling of Comilling for Efficient Integration into Continuous Process — ***Nirupaplava Metta***, ***Marianthi Ierapetritou***, ***Rohit Ramachandran***

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(138) CO_2 Use and Reuse
Monday, Oct 30, 12:30 PM
MCC, 200C

Lynn Brickett, Chair
Rameshwar Srivastava, Co-Chair

Sponsored by:
Advances in Fossil Energy R&D

12:30 Paper 138a: The U.S. Department of Energy's R&D Program for Carbon Use and Reuse — ***Lynn Brickett***

12:52 Paper 138b: Design of New Bimetallic Catalysts for More Selective CO_2 Hydrogenation to Olefins and Methanol — ***Chunshan Song***

1:14 Paper 138c: Direct Carbonation of $Ca(OH)_2$ Using Liquid and Supercritical CO_2 — ***Daniel Klingenberg***, *Ali Zolghadr, Joseph Biernacki*

1:36 Paper 138d: CO_2 Upcycling via Mineralization of a Carbonate-Based Construction Material: Processing-Property Relationships of Co_2Ncrete™ — ***Gabriel Falzone***, *Bu Wang, Zhenhua Wei, Joseph Gall, Yiu Shun Wong, Gaurav Sant*

1:58 Paper 138e: CO_2 Conversion to Fuels and Chemicals Through Microbial Electrolysis Cells — ***Yanna Liang***, *Hannah Giang, Ian Suni, Ji Zhang*

2:20 Paper 138f: High-Selectivity Gas Fermentation of CO_2 to Ethanol — ***Allan H. Gao***, *Robert Conrado, Bruce Li, Christophe Mihalcea, Sean D. Simpson*

2:42 Paper 138g: Role of Nitrogen Addition to Reduced Graphene Oxide–TiO_2 Nanocomposites in Enhancing CO_2 Photoreduction — ***Yao Nie,*** *Liang-Yi Lin, Wei-Ning Wang, Pratim Biswas*

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(139) Dynamics and Modeling of Particulate Systems II
Monday, Oct 30, 12:30 PM
MCC, 200J

Joerg Theuerkauf, Chair
Maulik Mehta, Co-Chair

Sponsored by:
Solids Flow, Handling and Processing

12:30 Paper 139a: A Unified Theory for the Solid Stresses in Particle-Laden Flow — ***Raffaella Ocone***, *Yassir Makkawi, Xi Yu*

12:49 Paper 139b: Numerical Determination of Contact Laws for Compressible Particles — ***Ben Edmans***, *Csaba Sinka*

1:08 Paper 139c: Determining Collisional Dissipation Rate for Elongated Rods with Friction Using Homogeneous Cooling System Simulations — ***Kevin E. Buettner***, *Yu Guo, Jennifer Sinclair Curtis*

1:27 Paper 139d: An Integrated Workflow for Numerical Generation and Meshing of Packed Beds of Non-Spherical Particles — ***Behnam Partopour***, *Anthony G. Dixon*

1:46 Paper 139e: Flow of Granular Materials in a Bladed Mixer: Effect of Particle and Process Parameters on Impeller Torque — ***Veerakiet Boonkanokwong***, *Rohan P. Frank, Brenda Remy, Johannes G. Khinast, Benjamin J. Glasser*

2:05 Paper 139f: Study of Spontaneous Structure Formation in Granular Systems Using DEM Framework — ***Jielin Yu***, *Chunliang Wu, Oladapo Ayeni, Krishnaswamy Nandakumar, Jyeshtharaj B. Joshi, Mayank Tyagi, Shankar Ghosh*

2:24 Paper 139g: Assessment of the Effect of Dairy Powder Properties on Lean-Phase Pneumatic Transport: A CFD-DEM Modelling Approach — *Akeem Olaleye,* ***Harry E. A. Van den Akker***

2:43 Paper 139h: Advances in Voidage Reconstruction Schemes for the Simulation of Dense Gas-Particle Flows — ***Stefan Radl***, *Maryam Askarishahi, Christoph Goniva*

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(140) Effects of Confinement on Molecular Properties
Monday, Oct 30, 12:30 PM
MCC, L100J

Liangliang Huang, Chair
Robert A. Riggleman, Co-Chair

Sponsored by:
Thermodynamics and Transport Properties

12:30 Paper 140a: Adsorption and Phase Behavior of Mixed Alkanes in Nano-Slit Graphite Pores: An iSAFT Application — ***Jinlu Liu***, *Dilip Asthagiri, Walter G. Chapman*

12:46 Paper 140b: Oscillation and Enhancement of Gas Solubility in Nanopores — ***Xiaochen Yu***, *Liangliang Huang, Shuangliang Zhao Sr., Honglai Liu, Keith E. Gubbins*

1:02 Paper 140c: Effect of Interaction Position on Molecular Transport and Separation Through a Multi-Site Nanopore — ***Shaghayegh Agah,*** *Matteo Pasquali, Anatoly Kolomeisky*

1:18 Paper 140d: Strain-Induced Topological Defects and Configurational Transitions in Liquid Crystals — ***Monirosadat Sadati***, *Jose Martinez-Gonzalez, Khia Kurtenbach, Luis X. de Pablo, Harrison Shapiro, Samuel Morin, Ye Zhou, Juan de Pablo*

1:34 Paper 140e: Alkyl Chain Length and Nanoconfinement Effects on Dynamics of Imidazolium-Based Ionic Liquids — ***Yu Zhang***, *Naresh C. Otsi, Eugene Mamontov, Peter T. Cummings*

1:50 Paper 140f: A Molecular Simulation Study on CO_2 and a Deep Eutectic Solvent in Slit Nanopores — ***Yan Shen,*** *Francisco R. Hung*

2:06 Paper 140g: Molecular Simulation of Methane Adsorption Behavior in Nanopores for Shale Gas Development: With Comparison Between Graphite and Kerogen Models — *Jinrong Cao,* ***Yunfeng Liang***, *Yoshihiro Masuda, Hiroaki Koga, Hiroyuki Tanaka, Toshifumi Matsuoka*

2:22 Paper 140h: Brownian Dynamics Simulations on Spontaneous Extension of DNA on Cationic Lipid Bilayers Along Grooved Structures — ***Chang Ming-Yi***, *Ching-Kuan Wang, Chih-Chen Hsieh*

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(141) Electrocatalysis and Photoelectrocatalysis II: HER/HOR
Monday, Oct 30, 12:30 PM
MCC, L100D

Yijin Kang, Chair
Gang Wu, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

12:30 Welcoming Remarks

12:31 Paper 141a: Design of Advanced Nanomaterials for Electrocatalysis — ***Yijin Kang***

12:49 Paper 141b: Transition Metal Oxides and Carbides as Electrocatalysts — ***Aleksandra Vojvodic***

1:07 Paper 141c: Layered Hybrid Structure of Cobalt/N-Doped Carbon Derived from Metal-Organic Frameworks for Electrocatalytic Hydrogen Evolution — ***Tan Huang***, *Jong-Min Lee*

1:25 Paper 141d: Comparison of Hydroxide-Mediated and Direct Mechanisms for Alkaline Hydrogen Electrocatalysis — *Saad Intikhab, Jennifer Gallup, Joshua Snyder,* ***Maureen H. Tang***

1:43 Break

1:48 Paper 141e: Alkaline Hydrogen Evolution from Ni–Mo Intermetallics with High Mo Content — ***James R. McKone***, *Peter Csernica, Francis J. DiSalvo, Héctor D. Abruña*

2:06 Paper 141f: Increased Photocatalytic Activity of TiO_2 Nanoparticles with Defects for Sustainable Hydrogen Production — ***Ashley M. Pennington***, *Fuat E. Celik*

2:24 Paper 141g: Transition Metal Nitride Core-Noble Metal-Shell Nanoparticles as Highly CO-Tolerant Catalysts — ***Aaron Garg***, *Maria Milina, Madelyn Ball, Sean T. Hunt, James A. Dumesic, Yuriy Román-Leshkov*

2:42 Paper 141h: Understanding the Electrochemical Behavior of a Thin, Flexible Micro Fuel Cell — ***Seyed Reza Mahmoodi***, *Matthew Mayer, Ronald S. Besser*

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(142) Emerging Tools and Enabling Technologies in Synthetic Biology
Monday, Oct 30, 12:30 PM
MCC, 207A/B

Anushree Chatterjee, Chair
Yongku Cho, Co-Chair
Kang Wu, Co-Chair
Cong T. Trinh, Co-Chair

Sponsored by: Bioengineering

12:30 Paper 142a: Using Synthetic Biology to Engineer Epistasis to Deter Bacterial Adaptation — ***Peter Otoupal***, ***Anushree Chatterjee***

12:48 Paper 142b: Programmable Control of CRISPR-Cas9 Systems by Engineering SgRNA as Toehold-Switchable Riboregulators — ***Kay Siu***, *Wilfred Chen*

1:06 Paper 142c: Engineering Post-Translational Proofreading to Discriminate Non-Standard Amino Acids — ***Aditya M. Kunjapur***, *Devon Stork, Erkin Kuru, Matthieu Landon, Oscar Vargas-Rodriguez, Dieter Söll, George M. Church*

1:24 Paper 142d: Developing Robust, Environmentally Responsive Genetic Circuits for Real-World Applications — *Tatenda Shopera, Allison Hoynes-O'Connor, Young Je Lee, Austin Rottinghaus,* ***Tae Seok Moon***

1:42 Paper 142e: RNA-Aptamer-in-Droplet (RAPID) High-Throughput Screening for Secretory Phenotypes — ***James M. Wagner***, *Joseph Abatemarco, Maen Sarhan, Jyun-Liang Lin, Leqian Liu, Shuo-Fu Yuan, Adam Abate, Hal Alper*

2:00 Paper 142f: Enabling Microbial Cell Factories: Synthetic Biology Tools for Efficient Pathway Assembly and Integration — ***Ee Lui Ang***, *Jing Liang, Zihe Liu, Shuobo Shi, Youyun Liang, Mingzi M. Zhang, Xi Zhi Low, Huimin Zhao*

2:18 Paper 142g: Biology by Design: Emerging Tools in Cell-Free Synthetic Biology — ***Michael C. Jewett***

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(143) Engineering in Cancer Biology and Therapy II
Monday, Oct 30, 12:30 PM
MCC, 208B

Korkut Uygun, Chair
Mark P. Styczynski, Co-Chair

Sponsored by:
Engineering Fundamentals in Life Science

12:30 Paper 143a: Single-Particle Tracking of Oncogenic Microvesicle Interactions with Planar, Supported Stem Cell Bilayers — ***Han-Yuan Liu***, *Johana Uribe, Lakshmi Nathan, Claudia Fischbach-Teschl, Susan Daniel*

12:48 Paper 143b: Label-Free Interference-Based Quantitative Study of Filopodia-Like Structures in Cancer Cells of Different Metastatic Potential — ***Jose C. Contreras-Naranjo***, *Arul Jayaraman, Victor M. Ugaz*

1:06 Paper 143c: A Genetically Encoded Toolbox for Glycocalyx Engineering: Tunable Control of Cell Adhesion, Survival, and Cancer Cell Behaviors — ***Carolyn Shurer***, *Marshall Colville, Vivek Gupta, Shelby Head, FuiBoon Kai, Jonathon Lakins, Matthew Paszek*

1:24 Paper 143d: Quantification of the Effects of High Shear Stresses on Single Circulating Tumor Cells Using a Microfluidic Device — *Grant Landwehr, Sharif M. Rahman, Jacob Pettigrew, Ursula L. Triantafillu, Yonghyun (John) Kim,* ***Adam Melvin***

1:42 Paper 143e: Investigating the Effects of Cold Atmospheric Plasma on Cervical Cancer — ***Nicole J. Sova, Yonry Zhu***, *Ariel L. Lanier, Amir M. Farnoud, David Burnette, Monica M. Burdick*

2:00 Paper 143f: Targeted and Controlled Combination Therapy Using siRNA and Resveratrol for Inducing Leukemic Cell Apoptosis — ***Thikrayat Al-Attar***, *Abdurizzagh Khalf, Sundararajan V. Madihally*

2:18 Paper 143g: Nanostructured Platforms to Evaluate Cell Migration-Microenvironment Interactions in Glioma — ***Jessica O. Winter***

(144) Environmental Division Awards and Honors (Invited Talks)
Monday, Oct 30, 12:30 PM
MCC, 102E

V. Faye McNeill, Chair
Panagiotis Smirniotis, Co-Chair
Leslie M. Shor, Co-Chair

Sponsored by: Environmental Division

12:30 Paper 144a: Lawrence K. Cecil Award Lecture: Environmental Aspects in the Utilization of Fossil Fuels — ***JoAnn S. Lighty***

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(145) Free Forum on Engineering Education: Junior and Senior Years I
Monday, Oct 30, 12:30 PM
MCC, 205C

Kevin Hadley, Co-Chair
Randy D. Weinstein, Co-Chair
Jonathan E. Wenzel, Co-Chair

Sponsored by:
Undergraduate Education

12:30 Paper 145a: Mixing Experiences — ***Polly R. Piergiovanni***

12:48 Paper 145b: Large Changes in the OKState Unit Operations Lab — ***Clint P. Aichele***, *Gina Morris, Kristi Dickey, Brad Rowland, Shelley Potter, Michael R. Resetarits*

1:06 Paper 145c: Pharmaceutical Engineering: Curricular Integration and a Liberal Arts Perspective on a Chemical Engineering Elective — ***Ryan C. Snyder***

1:24 Paper 145d: Updating the Process Controls and Dynamics Course for the 21st Century — ***Wayne S. Seames***

1:42 Paper 145e: Safety Considerations When Designing a New Chemical Engineering Research Laboratory — ***William J. R. Gilbert***, *Mark B. Shiflett*

2:00 Paper 145f: Chemical Engineering Laboratory at the University of Kansas — ***David Griffin***, *Mark B. Shiflett*

2:18 Paper 145g: Biodiesel Production as a Case Study in Chemical Engineering: Senior Laboratory at University of Delaware — ***Robert J. Lovelett***, *Matthew Alba, Weihua Deng*

2:36 Paper 145h: Laboratory and Design Projects in Energy Sustainability Based on Industrial Operations and Data (Power Plants, Sugar Mills, Pilot Plants) — ***Kerry M. Dooley,*** *F. Carl Knopf, Jaren Lee*

(146) Fundamentals of Fluidization II
Monday, Oct 30, 12:30 PM
MCC, 200I

S. B. Reddy Karri, Chair
Hidehiro Kamiya, Co-Chair

Sponsored by:
Fluidization and Fluid-Particle Systems

12:30 Paper 146a: Hydrodynamics of Sound-Assisted Fluidization of Rigid-Microsized Powder — ***Parimanan Cherntongchai***

12:47 Paper 146b: Behaviour of Fine Particles in a Cold Plasma-Enhanced Spouted Bed — ***Baiqiang Zhang***, *Nobusuke Kobayashi, Yoshinori Itaya*

1:04 Paper 146c: Magnetic Resonance Imaging of Wet Fluidization — ***Christopher M. Boyce***, *Alexander Penn, Klaas P. Pruessmann, Christoph Mueller*

1:21 Paper 146d: CFD-DEM Modeling the Effect of Column Size and Bed Height on Minimum Fluidization Velocity in Micro Fluidized Beds with Geldart B Particles — ***Yupeng Xu,*** *Tingwen Li, Jordan Musser, Xiaoxing Liu, Guangwen Xu, William A. Rogers*

1:38 Paper 146e: DEM and Experimental Study of the Flow of Wet Granular Assemblies Under Dynamic Conditions — ***Jarray Ahmed***, *Magnanimo Vanessa, Stefan Luding*

1:55 Paper 146f: A Numerical Algorithm for Simulating Dense Polydisperse Gas-Particle Flows Using a Mass-Velocity Quadrature-Based Moment Method — ***Bo Kong***, *Rodney O. Fox*

2:12 Paper 146g: Effects of Wall Boundary Conditions on 3D Simulation of Pseudo-Two-Dimensional Fluidized Beds Using Dense Discrete Phase Model (DDPM) — ***Abolhasan Hashemisohi***, *Abloghasem Shahbazi, Lijun Wang*

2:29 Paper 146h: RANS Modeling of Cluster-Induced Turbulence in Particle-Laden Channel Flow — ***Michael Baker***, *Rodney O. Fox, Bo Kong, Olivier Desjardins, Jesse Capecelatro*

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(147) Fundamental, Theory, and Model Development — In Honor of Keith Gubbins's 80th Birthday II (Invited Talks)
Monday, Oct 30, 12:30 PM
MCC, L100H

Erik E. Santiso, Chair
Liangliang Huang, Co-Chair

Sponsored by:
Computational Molecular Science and Engineering Forum

12:30 Paper 147a: Metastable Phase Transitions — ***Pablo G. Debenedetti***

12:55 Paper 147b: Computational Investigation of Multipolar Colloidal Particle — *David M. Rutkowski, Ryan C. Maloney, Orlin D. Velev, Sabine H. L. Klapp,* ***Carol K. Hall***

1:20 Paper 147c: Interfacial Tensions from SAFT: Connecting Equations of State to Molecular Simulations — ***Erich A. Müller***

1:45 Paper 147d: Generalized Gibbs Free Energy of Confined Nanoparticles — ***Xiaohua Lu***

2:10 Paper 147e: Molecular Modeling of Polymeric Systems — ***Coray M. Colina***

2:35 Paper 147f: Effect and Regulation of Surface Wettability on Molecular Transport and Reaction — ***Shuangliang Zhao Sr.***, *Honglai Liu*

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(148) Hydrodynamics of Biological Systems
Monday, Oct 30, 12:30 PM
Hilton, Marquette I/II/III/VIII/IX

F. C. MacKintosh, Chair
Kelly M. Schultz, Co-Chair

Sponsored by: Fluid Mechanics

12:30 Paper 148a: Dynamics of Collective Endothelial Cell Migration in Response to Fluid Shear Stress — ***Alexander Dunn***

1:00 Paper 148b: Rupture of Cancer Cells Under Microcirculatory Conditions — *Nabiollah Kamyabi,* ***Siva A. Vanapalli***

1:15 Paper 148c: Transport of Nanoparticles in the Brain — *Justin Rosch, C. B. Schaffer,* ***William L. Olbricht***

1:30 Paper 148d: Towards Understanding Nanoparticle Diffusion in Synovial Fluid Analogues — ***Mythreyi Unni***, *Lorena Maldonado-Camargo, Kyle Allen, Carlos Rinaldi*

1:45 Paper 148e: Diffusion of Concentrated Macromolecules Within Living Cells — ***Jiyuan Li***, *Xikai Jiang, Juan Hernandez-Ortiz, Olle G. Heinonen, Juan de Pablo*

2:00 Paper 148f: Platelet Margination, Adhesion, and Activation in Secondary Flows Are Necessary for Thrombus Propagation in an *In-Vitro* Model of Venous Thrombosis — ***Marcus Lehmann***, *Patrick Krohl, Keith B. Neeves*

2:15 Paper 148g: The Importance of Rheology in Blood Flow Modeling — ***Jeffrey S. Horner***, *Norman J. Wagner, Antony N. Beris, Donna S. Woulfe*

2:30 Paper 148h: *In Vitro* Measurement and Modelling of Platelet Adhesion on Von-Willebrand-Factor-Coated Surfaces in Channel Flow — ***Qin M. Qi***, *Irene K. Oglesby, Jonathan Cowman, Antonio J. Ricco, Dermot Kenny, Eric S. G. Shaqfeh*

2:45 Paper 148i: A Novel Viscoelastic Thrombogenesis Model from High-Performance Lattice Boltzmann Method Yield-Stress Calculations Based on Intravital Images of Clot Formation in Live Mice — ***Vishnu Deep Chandran***, *Olufemi Kadri, Roman Voronov*

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(149) In Honor of Bill Koros I
Monday, Oct 30, 12:30 PM
MCC, M100H

Ryan Lively, Chair
Benny D. Freeman, Co-Chair
Dhaval Bhandari, Co-Chair

Sponsored by:
Membrane-Based Separations

12:30 Paper 149a: Mixed-Matrix Membranes Based on Polymers of Intrinsic Microporosity and Metal-Organic Frameworks for Gas Separation Applications — ***Ingo Pinnau***, *Xiaohua Ma, Ramy Swaidan, Chia-En Hsiung, Yingge Wang, Yu Han*

12:52 Paper 149b: Revolutionary Ultrathin Carbon Molecular Sieve Hollow Fiber Membranes — ***Chen Zhang***, *William J. Koros*

1:14 Paper 149c: Engineering the Performance of Carbon Molecular Sieve Membranes Through the Use of Oxygen Doping — ***Jason Williams***, *W. J. Koros, Graham Wentz*

1:36 Paper 149d: Enhanced Transport Properties of Metal-Organic Framework Mixed-Matrix Membranes for Gas Separation — ***Gongping Liu***, *Yang Liu, Jie Shen, Kuang Zhang, Chen Zhang, Shouliang Yi, William Koros, Wanqin Jin, Mohamed Eddaoudi, Valeriya Chernikova, Osama Shekhah, Youssef Belmabkhout*

1:58 Paper 149e: Developing Robust Membranes for Natural Gas Processing — ***Nitesh Bhuwania***, *Daniel Chinn*

2:20 Paper 149f: Carbon Molecular Sieve Membranes as Enablers for Organic Solvent Reverse Osmosis — ***Ryan Lively***

2:42 Paper 149g: Carbon Molecular Sieve Structure Development and Membrane Performance Relationships — ***Meha Rungta***, *Graham Wenz, William J. Koros*

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(150) In Honor of Dennis Prieve's Retirement II (Invited Talks)
Monday, Oct 30, 12:30 PM
MCC, M100B

Christopher L. Wirth, Chair
Jeffrey A. Fagan, Co-Chair
Robert D. Tilton, Co-Chair

Sponsored by: Interfacial Phenomena

12:30 Welcoming Remarks

12:33 Paper 150a: Determination of the Zeta Potential of Planar Solids in Nonpolar Liquids — ***Paul J. Sides***, *Dennis Prieve, Benjamin A. Yezer*

12:51 Paper 150b: Toward Simulation-Based Design of Particle Handling Processes — ***Jennifer Sinclair Curtis***

1:09 Paper 150c: Sustainable Electrocatalytic Water Splitting with Earth-Abundant Materials — *Hao Yuan, Richard Lunt,* ***Robert Y. Ofoli****i*

1:27 Paper 150d: Human Tear Production from Capillary Wicking Dynamics — ***Clayton J. Radke***

1:45 Paper 150e: Structure, Elasticity, and Non-Equilibrium State Diagram of Depletion Gels — ***Eric M. Furst***

2:03 Paper 150f: Harnessing Solvation Forces for Dispersing Colloids in Ionic Liquids with Application in Human Exploration of Space — *Jingsi Gao,* ***Norman Wagner***

2:21 Paper 150g: Control of Interfacial Phase Separation by Electro-Autocatalysis — ***Martin Z. Bazant***

2:39 Paper 150h: Reduction of Particle Jamming in Abrasive Slurries — *Aditya A. Salunkhe, René M. Overney,* ***John C. Berg***

2:57 Concluding Remarks

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(151) In Honor of Martin Yarmush II (Invited Talks)
Monday, Oct 30, 12:30 PM
MCC, 208C/D

Kyongbum Lee, Chair
Charles Roth, Co-Chair

Sponsored by:
Food, Pharmaceutical & Bioengineering Division

12:30 Paper 151a: Human *In Vitro* Models to Improve Preclinical Testing of Drugs — ***Michael L. Shuler***

12:55 Paper 151b: Invited Talk — ***Kostas Konstantopoulos***

1:20 Paper 151c: CAR-T Manufacturing: Delivering on the Promise of a Transformational Therapy — ***Gregory Rusotti***

1:45 Paper 151d: The Importance of Thinking Big in Academia — ***Scott Banta***

2:10 Paper 151e: Plasmonic Nanomaterials for Tissue Sealing and Radiation Dosimetry — ***Kaushal Rege***

2:35 Paper 151f: Invited Talk — ***Ipsita Banerjee***

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(152) In Honor of Stuart W. Churchill I (Invited Talks)
Monday, Oct 30, 12:30 PM
MCC, 101E

Warren D. Seider, Chair
Peter Lederman, Co-Chair

Sponsored by:
Transport and Energy Processes

12:30 Introductory Remarks

12:35 Paper 152a: Digital Alchemy for Assembly Engineering — ***Sharon C. Glotzer***

1:05 Paper 152b: Improved Algebraic, Numerical, and Graphical Representations in Fluid Mechanics — ***Stuart W. Churchill****, James C. Hill*

1:35 Paper 152c: The Scaling of Turbulence near the Wall and the Churchill Turbulent Flux Correlation: Insights with Lagrangian Simulations — ***Dimitrios V. Papavassiliou****, Quoc T. Nguyen, Chiranth Srinivasan*

2:05 Paper 152d: Flow Boiling Using a Piranha Pin Fin Heat Sink — ***Cory Woodcock****, Xiangfei Yu, Yoav Peles, Joel L. Plawsky*

2:35 Paper 152e: Transport Problems in the Spirit of Stuart Churchill for Teaching and Research at the University of Michigan — ***Ronald G. Larson****, Claudio Vilas Boas Favero*

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(153) In Honor of the 2016 Wilhelm Award Winner II (Invited Talks)
Monday, Oct 30, 12:30 PM
MCC, L100A

John R. Regalbuto, Chair
Jonas Baltrusaitis, Co-Chair
Israel E. Wachs, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

12:30 Paper 153a: Understanding the Mechanism and Kinetics of Reactions Catalyzed by Metal Oxides — ***Alexis T. Bell***

12:55 Paper 153b: Controlling Strain and Ligand Effects in Nanoparticle Catalysis by Alloying: Novel Alloys for Electrochemical Oxygen Reduction Reaction — ***Suljo Linic***

1:20 Paper 153c: A Synopsis of the Production of Propylene via Oxidative Dehydrogenation of Propane: How Far from Its Commercial Implementation? — ***Carlos A. Carrero***

1:45 Paper 153d: Insights into the Molecular Structure of Sulfated Mixed Metal Oxide Catalysts via Vibrational Spectroscopy — ***George Tsilomelekis***

2:10 Paper 153e: Supported Metal Oxides as Model Oxide Catalysts — ***Israel Wachs***

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(154) Jumpstart Your Teaching! Small Teaching Ideas for Course Improvement
Monday, Oct 30, 12:30 PM
MCC, 205D

Daniel Lepek, Co-Chair
Daniel Anastasio, Co-Chair

Sponsored by:
Undergraduate Education

12:30 Paper 154a: Generating Student-Created Exam Solutions: An Activity for Repetition and Reflection — ***Matthew Liberatore***

12:48 Paper 154b: A Student-Created, Open-Access, Living Textbook — *Shelly R. Peyton,* ***Sarah L. Perry****, Sualyneth Galarza*

1:06 Paper 154c: Adapting Best Practices from Middle School Classrooms to Chemical Engineering Courses — ***Amanda Simson***

1:24 Paper 154d: Giving a Grade to Teamwork — ***Jennifer Cole***

1:42 Paper 154e: Laboratory Measurement: Much Ado About Everything — ***Jacob H. Arredondo****, Timothy Threatt, Jonathan H. Worstell*

2:00 Paper 154f: Aligning the Unit Operations Laboratory and the National Academy's Grand Challenges — ***Tracy Carter****, Abigail Koppes, Lucas J. Landherr, Ronald J. Willey*

2:18 Paper 154g: No More Death by PowerPoint! Using the Assertion-Evidence Technical Presentation Model in a ChE Unit Operations Course — ***Matthew Cooper***

2:36 Panel Discussion

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(155) MAC Chemical Engineering Forum (Invited Talks)
Monday, Oct 30, 12:30 PM
MCC, 101F

Emmanuel Dada, Chair

Sponsored by:
Minority Affairs Committee

12:30 Introductory Remarks from MAC Eminent Chemical Engineers Award Committee

12:40 Paper 155a: Smart Manufacturing in the Automobile Industry — ***Alicia Boler-Davis***

1:10 Paper 155b: Smart Manufacturing in Chemical Industries — ***Emmanuel Dada****, Timothy Odi*

1:40 Paper 155c: Innovations in Chemical Engineering: Automation of the Factories of the Future and the Impact of Internet of Things (IoT) from the Control of the machinery in factories to Home Appliances — ***Thomas Mensah***

2:10 Paper 155d: Reversing the Tide in Science, Engineering, Technology, and Science (STEM): Academically Gifted African American Students in Historically Black Colleges and Universities (HBCU) — ***Felecia Nave***

2:30 Paper 155e: Blacks in Science, Engineering and Medicine: Struggles that Continue, Struggles that are Growing, and Possible Solutions — ***Cato Laurencin***

2:50 Presentation of Awards, T. Bond Calloway, Jr., AIChE President

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(156) Materials and Processes for Thermo-, Electro- and Photo-Chemical Energy Storage
Monday, Oct 30, 12:30 PM
MCC, 103B

Wei Liu, Chair
Jian Liu, Co-Chair
Anthony Shoji Hall, Co-Chair

Sponsored by:
Innovations of Green Process Engineering for Sustainable Energy and Environment

12:30 Paper 156a: Low-Temperature Synthesis of NH_3 from Air and Water for Electrical Energy Storage — ***Wei Liu***

12:55 Paper 156b: Thermochemical Storage of Solar Energy via Metal Oxide/Metal Sulfate Water Splitting Cycle — ***Rahul Bhosale****, Parag N. Sutar, Gorakshnath Takalkar*

1:20 Paper 156c: 2017 Topical Conference: Innovations of Green Process Engineering for Sustainable Energy and Environment — ***Anthony Shoji Ha****ll, Du Sun*

1:45 Paper 156d: sCO_2 Power Cycles with Integrated Thermochemical Energy Storage Using an MgO-Based sCO_2 Sorbent in Direct Contact with Working Fluid for Grid Energy Storage Applications — ***Andrew Muto****, Kevin McCabe, Daniel Real*

2:10 Paper 156e: Solar Thermochemical CO_2 Splitting Using Redox Cycles of Cr-Doped Mn-Based Perovskites — ***Alfonso J. Carrillo****, Thierry Moser, Alexander H. Bork, Jennifer L. M. Rupp*

2:35 Paper 156f: Study on the Performance of Fe_2O_3-MgO/Al_2O_3 as the Oxygen Carrier in Chemical-Looping Hydrogen Generation — ***Hao Liang***

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(157) Materials for Electrochemical Energy II
Monday, Oct 30, 12:30 PM
MCC, 210A/B

Gang Wu, Chair
Juchen Guo, Co-Chair

Sponsored by:
Electronics and Photonics

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(158) Membranes for Bioseparations
Monday, Oct 30, 12:30 PM
MCC, M100D

Heather C. S. Chenette, Chair
Stephen M. Ritchie, Co-Chair

Sponsored by: Bio Separations

12:30 Break

1:00 Paper 158b: Screening, Purification and Concentration of Membrane Proteins — ***Hasin Feroz****, Andrew L. Zydney, Manish Kumar*

1:30 Paper 158c: The Effects of Filtration Condition on Virus Clearance — ***Namila Khereid****, Rong Fan, S. Ranil Wickramasinghe, Xianghong Qian*

2:00 Paper 158d: Modification of Polycarbonate Membranes with EDC/NHS Coupling: The Impact of Electrostatic Particle-Pore Interactions on Rejection — *Armin Delavari, Daniel Breite,* ***Ruth E. Baltus****, Agnes Schulze*

2:30 Paper 158e: Smart Nanogel-Containing Membranes in Microchip for Temperature- and Ethanol-Responsive Permeability Regulation — ***Wei Wang****, Rui Xie, Xiao-Jie Ju, Zhuang Liu, Liang-Yin Chu*

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(159) Membrane Tutorial (Invited Talks)
Monday, Oct 30, 12:30 PM
MCC, M100I

John Pellegrino, Co-Chair
William B. Krantz, Co-Chair
Jeffrey R. McCutcheon, Co-Chair

Sponsored by:
Membrane-Based Separations

12:30 Paper 159a: Membrane Water Treatment: Process Design Considerations and Economics — ***Leaelaf M. Hailemariam***

12:55 Paper 159b: Molecular Simulations to Inform Polymeric Membrane Science and Technology — ***Richard M. Lueptow***

1:20 Paper 159c: Tutorial on Membrane Separations Technology for the Biopharmaceutical Industry — ***Andrew Zydney***

1:45 Paper 159d: A Methodology for the Evaluation of Membrane Robustness and Lifetime — ***C. J. Kurth***

2:10 Paper 159e: Membrane Processes Utilizing Coupled Heat and Moisture Transfer — ***Jason Woods***

2:35 Paper 159f: Transport Processes in Batteries: A Synergistic Research Direction for Membrane Scientists — ***Bryan D. McCloskey***

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(160) Microfluidic and Nanoscale Flows: Multiphase and Fields
Monday, Oct 30, 12:30 PM
Hilton, Conrad D

Cari S. Dutcher, Chair
Siva A. Vanapalli, Co-Chair

Sponsored by: Fluid Mechanics

12:30 Paper 160a: Layered Fluid-Fluid Interfaces Confined in Microfluidics — *Bruno Pinho,* ***Ryan L. Hartman***

12:45 Paper 160b: Focused DC and AC Electric Fields at Conic Pipettes: Nanoscale Thermal Hotspot and Nano-Droplet Generation with Universal Scalings — ***Hsueh-Chia Chang****, Zehao Pan*

1:00 Paper 160c: Real-Time Monitoring of Complex Multiphase Behavior in a High-Pressure, High-Temperature Microfluidic Chip — ***R. M. Ripken****, J. G. E. Gardeniers, S. Le Gac*

1:15 Paper 160d: Motion of a Deformable Drop in Microchannels of Complex Shape — ***Robert H. Davis****, Rocio Navarro, Alexander Zinchenko*

1:30 Paper 160e: Coupled Level Set Volume of Fluid (CLSVOF) Study on Droplet Formation and Breakup Mechanism in a Flow-Focusing Device — ***Somasekhara Goud Sontti****, Arnab Atta*

1:45 Paper 160f: Microfluidic Device for the Continuous Measurement of Viscosity — *Yunzi Li,* ***Sarah E. Mena****, Kevin R. Ward, Mark A. Burns*

2:00 Paper 160g: Simple Algebraic Formulas for the Practical Interpretation of Mercury Porosimetry Data — ***Zongyu Gu****, Martin Z. Bazant*

2:15 Paper 160h: A Microfluidic Platform to Measure Dynamic Interfacial Tension of Complex Fluid Systems — ***Shweta Narayan****, Davis B. Moravec, Brad G. Hauser, Andrew J. Dallas, Cari S. Dutcher*

2:30 Paper 160i: Controlled Liquid Entrapment Through Photo-Patterned Obstacles and Patterned Surfaces — ***Ankur Gupta****, Hyundo Lee, T. Alan Hatton, Patrick S. Doyle*

2:45 Paper 160j: Tears of Wine — *Prerana Rathore,* ***Vivek Sharma***

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(161) Mixing in Multi-Phase Systems
Monday, Oct 30, 12:30 PM
MCC, 102D

Richard V. Calabrese, Chair
Eric E. Janz, Co-Chair

Sponsored by:
North American Mixing Forum

12:30 Paper 161a: The Development of a Correlation for Solid-Liquid Cloud Height in Mechanical Agitated Vessels — ***Robert P. Hesketh****, Arthur W. Etchells III*

12:49 Paper 161b: Impeller Power Draw During Turbulent Operation in Liquid-Solid Suspensions — ***Kevin Myers****, Eric E. Janz*

1:08 Paper 161c: Novel Experimental Method for the Determination of the Minimum Agitation Speed for Solids Suspension in Flat-Bottomed Stirred-Tank Reactors — *Shriarjun Shastry,* ***Piero M. Armenante***

1:27 Paper 161d: Simulating Solid Suspension in Stirred Vessels with a Fully Coupled CFD-DEM Algorithm — *Oleh Baran, Ravindra Aglave, Simon Lo,* ***Thomas Eppinger***

1:46 Paper 161e: Understanding Particle Attrition in Agitated 3-Phase Aerated Slurry Reactors — ***Justin Walker****, Mark Joswiak, Patrick McGough*

2:05 Paper 161f: A Unifying Framework for Mass Transfer Dynamics in Gas–Liquid Segmented Flow in a Circular Tube — ***Ghata Nirmal****, Thomas F. Leary, Arun Ramachandran*

2:24 Paper 161g: Phase Inversion of a Solid-Stabilized Emulsion: Effect of Particle Concentration — *Bing Wan,* ***Louis Fradette***

2:43 Paper 161h: A Eulerian-Lagrangian Hybrid Model for the Simulation of the Droplet Size Distribution of Liquid-Liquid Emulsions in Stirred-Tank Reactors — *Reza Farzad,* ***Simon Schneiderbauer***

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(162) Model-Based Integrated Design of Pharmaceutical Drug Product Processes
Monday, Oct 30, 12:30 PM
MCC, 205A/B

Brendon G. Ricart, Chair
Nima Yazdanpanah, Co-Chair

Sponsored by:
Pharmaceutical Discovery, Development and Manufacturing Forum

12:30 Paper 162a: A Compartmentalized, Numerical Model of Continuous Blending — ***Pongpumin Bunchatheeravate****, Joseph W. Bullard, Steven Dale, Greg Connelly, Marcus O'Mahony*

12:52 Paper 162b: Impact of Raw Material and Blend Properties on the Screw Feeding, Continuous Blending and Tableting Unit Operation of an Integrated Continuous Direct Compression Platform — ***Bernd Van Snick****, Valérie Vanhoorne, Maxim Verstraeten, Jens Dhondt, Giustino Di Pretoro, Thomas De Beer, Chris Vervaet*

1:14 Paper 162c: Feeder Characterization and Model Development Accounting for Incoming Material Properties — ***M. Sebastian Escotet-Espinoza****, Glinka Cathy Pereira, Andrés D. Román-Ospino, Fernando J. Muzzio, Marianthi Ierapetritou*

1:36 Paper 162d: Disintegration and Dissolution Modeling for Accelerated Drug Product Process Development — ***Pedro Valente****, Slavomira Doktorovova, Nuno Enes, João Henriques, Paulo Lino, Inês Lopes, Nuno Neves, Mafalda Paiva, Tiago Porfírio, João Vicente, Márcio Temtem*

1:58 Paper 162e: Modeling of Flow and Drying of Aqueous Polymer Coatings on Porous Pharmaceutical Tablets — ***Charalampos Christodoulou****, Eva Sørensen, Salvador García-Muñoz, Luca Mazzei*

2:20 Paper 162f: Modelling and Simulation Efforts in Scale-Up and Characterisation of Semi-Solid Dosage Forms — ***Saurav S. Rath***, *Birendra K. David, RaviChandra Palaparthi*

2:42 Paper 162g: Dissolution Kinetics Modelling of a BCS Class II Active Pharmaceutical Ingredient — ***Yuan Gao***, *Brian Glennon, Yunliang He, Guangyang Hou, Philip Donnellan*

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(163) Molecular Simulation and Modeling of Complex Molecules
Monday, Oct 30, 12:30 PM
MCC, L100I

Steven M. Abel, Chair
Mark J. Uline, Co-Chair

Sponsored by:
Thermodynamics and Transport Properties

12:30 Paper 163a: Kinetics of (Un) Binding Between DNA-Functionalized Particles Using a Coarse-Grained Model with Explicit Nucleotide Representation — ***Tiara Ann Maula***, *Jeetain Mittal*

12:48 Paper 163b: Multiscale Molecular Modeling of Fluorescent Organic Nanotubes — ***Arthur Gonzales***, *Belete Legesse, Takeshi Yamazaki, Hicham Fenniri*

1:06 Paper 163c: Hydration Structure and Dynamics of Poly(2-methacryloyloxyethyl phosphorylcholine) — ***Christoph Klein***, *William L. Roussell, Christopher R. Iacovella, Clare McCabe, Peter T. Cummings*

1:24 Paper 163d: Polyelectrolyte Interactions: Simulation and Theory — *Maria Sammalkorpi, Hanne Antila,* ***Paul R. Van Tassel***

1:42 Paper 163e: Modeling Solute and Solvent Distributions in Functionalized Dendrimers from iSAFT Density Functional Theory — ***Yuchong Zhang***, *Walter G. Chapman*

2:00 Paper 163f: Dependence of Relaxations and Mechanical Properties on Molecule Shape in Dissipative Particle Dynamics — ***Michael L. Greenfield***, *Claire A. Lemarchand, Jesper S. Hansen*

2:18 Paper 163g: Thermodynamics of Self-Assembly of Perylene Derivatives — *Jörg Baz,* ***Niels Hansen***

2:36 Paper 163h: A Molecular Dynamics Study of Actinide Nanoclusters — ***Ken Newcomb***, *Edward J. Maginn*

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(164) Nanomaterial Applications for Human Health and the Environment
Monday, Oct 30, 12:30 PM
MCC, 101D

Nastassja Lewinski, Chair
Yinlun Huang, Co-Chair
Cory Jensen, Co-Chair
Amitesh Saha, Co-Chair

Sponsored by: General

12:30 Paper 164a: Design and Redesign of Sustainable Engineered Nanomaterials — ***Christy L. Haynes***

12:48 Paper 164b: DNA Nanotechnology: A Promising Tool to Target Cancer — ***Efrosini Kokkoli***

1:06 Paper 164c: Functionalization of Iron Oxide Nanoparticles and the Impact on Reactive Oxygen Species Generation for Potential Cancer Treatment — ***Trang Mai***, *James Z. Hilt*

1:24 Paper 164d: Theranostic Nanovehicles for the Diagnosis and Treatment of Cerebrovascular Diseases — ***Karunya Kandimalla***

1:42 Paper 164e: Three-Dimensional Graphene-Based Microbarriers for Controlling Release and Reactivity in Colloidal Liquid Phases — ***Megan A. Creighton***, *Wenpeng Zhu, Finn van Krieken, Robert A. Petteruti, Huajian Gao, Robert Hurt*

2:00 Paper 164f: Nanostructured Materials for Sensitive and Selective NH_3 Detection — ***Yu Lei***

2:18 Paper 164g: Enhancing Microfluidic Capture of Circulating Tumor Cells Using Magnetic Nanoparticles — ***Mythreyi Unni***, *Jinling Zhang, Z. Hugh Fan, Carlos Rinaldi*

2:36 Paper 164h: Actuating Gold Nanoparticle Chemiresistor Sensitivity and Selectivity for Sensing Carbonyl Compounds in Air — *Zhenzhen Xie, Mandapati Raju, Michael H. Nantz,* ***Xiao-an Fu***

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(165) Nanomaterials for Biological Applications II
Monday, Oct 30, 12:30 PM
MCC, 200G

Anushree Chatterjee, Chair
Prashant Nagpal, Co-Chair

Sponsored by:
Nanomaterials for Applications in Energy and Biology

12:30 Paper 165a: Functionalization of Graphene by Using Protein Engineering — ***Abhishek Tyagi***, *Irfan Haider Abidi, Zhengtang Luo*

12:55 Paper 165b: Developing Precision Medicine Using Quantum Biology: Combining Quantum States, Surface Chemistry, and Microbiology — ***Prashant Nagpal***, *Colleen Courtney, Samuel Goodman, Anushree Chatterjee*

1:20 Break

1:45 Paper 165d: Nanoscale Size-Controlled Electrospun Composite Mats of Chitosan with Tungsten Disulfide Inorganic Nanotubes (INT-WS_2) — *Apostolos Baklavaridis,* ***Ioannis Zuburtikudis***, *Constantinos Panayiotou*

2:10 Paper 165e: Biodegradable Multilayered Nanofilms for Cell Isolation and Recovery — ***Wei Li***, *Ziye Dong, Caroline Ahrens*

2:35 Paper 165f: Ag/Cu Bimetallic Nanoparticle and Ion-Graphene Composites with Enhanced Antibacterial Performance — *Anna Perdikaki, Angeliki Galeou,* ***Georgios N. Karanikolos***

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(166) Nanomaterials Manufacturing
Monday, Oct 30, 12:30 PM
MCC, 212A/B

Hebab Quazi, Chair
Thomas Mensah, Co-Chair

Sponsored by:
Nanoscale Science and Engineering Forum

12:30 Paper 166a: Microwave-Initiated Nanomanufacturing Towards Energy Applications — *Shatila Sarwar, Jonathan Cook, Amit Nautiyal,* ***Xinyu Zhang***

12:48 Paper 166b: Separation of Double-Decker-Shaped Silsesquioxanes Condensed with Multiple Functional Groups — ***David Vogelsang***, *Parker Dunk, Robert Maleczka Jr., Andre Y. Lee*

1:06 Paper 166c: Colloidal Assembly by Capacitive Deionization — ***Rodrigo Guerra***, *Paul M. Chaikin*

1:24 Paper 166d: Continuous Flow Synthesis of Ni-Based Nano-Catalysts — ***Lu Wang***, *Emily Roberts, Richard Brutchey, Noah Malmstadt*

1:42 Paper 166e: Process Optimization for the Synthesis of Gold and Copper Nanoparticles from a Mixed Precursor Solution — ***Kathryn Dill***, *Mahmoud Moustafa, Christina Tang, Nastassja Lewinski*

2:00 Paper 166f: Novel Techniques for Production and Morphology Manipulation of MXene Nanosheets — *Wanmei Sun, Smit Shah, Touseef Habib, Miladin Radovic,* ***Micah Green***

2:18 Paper 166g: Cellulose-Assisted Combustion Synthesis of Nanoparticles for Catalytic Applications — ***Anand Kumar***, *Anchu Ashok, Md. Abdul Matin, Faris Tarlochan*

2:36 Paper 166h: Microgrids with Energy Storages: Technology Development and Commercialization of an Optimized, Reliable, Affordable, and Renewable Electricity Supply System for Communities Not Served by the Utilities — ***Hebab Quazi***, *Nick Tillmann, Hesan Quazi*

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(167) Nanomaterials Synthesis and Self-Assembly Strategies
Sunday, Oct 29, 3:30 PM
MCC, 211A

James Dorman, Chair

Sponsored by:
Electronics and Photonics

3:30 Paper 167a: Revealing Governing Mechanism in Directed Self-Assembly of sub-10 nm Particles with Single-Particle Resolution — *Zhen Luo,* ***Shafigh Mehraeen***

3:45 Paper 167b: Uniform Thinning of Cu-Fe-Ni-Co Nanowires and Kinetic Monte Carlo Simulation — *Xiaohua Geng,* ***Elizabeth Podlaha***

4:00 Paper 167c: Experimental Assessment of Nucleation Theory at the Molecular Level — ***Matthew A. Gebbie***, *Nicholas A. Melosh*

4:15 Paper 167d: Low-Voltage Electrophoretic Deposition of All-Inorganic CZTS Nanocrystals for Fabrication of Thin Films — ***Andrew D. Dillon***, *Mohammad Mehdi Taheri, Shawn Mengel, Subham Dastidar, Jason B. Baxter, Aaron T. Fafarman*

4:30 Paper 167e: Preferential Binding of Polyvinylpyrrolidone (PVP) Is Not Responsible for Shape Control in Ag Nanoparticle Synthesis — ***Zhifeng Chen***, *Ji Woong Chang, Choumini Balasanthiran, Robert M. Rioux*

4:45 Paper 167f Scalable Synthesis of Epitaxial, Oxidation-Proof Au@Ag Core-Shell Nanowires for Electronic and Photonic Applications — ***Ruoxue Yan***, *Yangzhi Zhu, Sanggon Kim, Peter Byrley*

5:00 Paper 167g: Synthesis of Bimetallic Alloy Nanoparticles Through the Visible Light–Mediated Reduction of a Bimetallic Oxide Precursor: Case Study of Ag-Pt Nanoparticle Synthesis — ***Umar Aslam***, *Suljo Linic*

5:15 Paper 167h: Dynamic Control of Gold Nanoparticle-Conjugated DNA Origami Templates — ***Abhilasha Dehankar***, *Joshua Johnson, Carlos E. Castro, Jessica O. Winter*

5:30 Paper 167i: 'One-Pot' Multiscale Templating of Interdigitated Bi-Modal Porous Carbon Supercapacitors — *Zheng Tian,* ***Megha Sharma***, *Mark A. Snyder*

5:45 Paper 167j: Combined Experimental and Theoretical Study of Hexagonal Boron Nitride Crystal Growth — ***Song Liu***, *Bin Liu, James H. Edgar*

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(168) PEM (Polymer Electrolyte Membrane or Proton Exchange Membrane) Fuel Cells, DMFC (Direct Methanol Fuel Cells), and Alkaline Fuel Cells
Monday, Oct 30, 12:30 PM
MCC, 200F

Yangchuan Xing, Chair

Sponsored by:
Transport and Energy Processes

12:30 Paper 168a: Session Keynote: Hydroxide-Conducting Aromatic Polymer Membranes and Their Applications in Fuel Cells — *Junyoung Han, Woo-Hyung Lee, Eun Joo Park, Jong Yeob Jeon, Angela Mohanty, Dong Won Shin, Chang Yeol Ryu,* ***Chulsung Bae***

12:55 Paper 168b: Session Keynote: Gas-Transport Limitations in Electrochemical Energy-Conversion Technologies — ***Adam Weber***

1:20 Paper 168c: Effect of Isopropyl Phosphate Incorporation on the Morphology and Transport Properties of Sulfonated Poly(styrene-isobutylene-styrene) Membranes — ***Eduardo Ruiz Colón***, *Maritza Perez Perez, David Suleiman*

1:45 Paper 168d: Experimental Measurements of Water Transport in Proton Exchange Membrane Fuel Cells via In-Situ Performance Testing and Ex-Situ Synchrotron X-Ray Radiography — *Logan Battrell, Erica Eggleton, Megan English, Lifeng Zhang,* ***Ryan Anderson***

2:10 Paper 168e: Synergy Between the Ether and the Sulfonic Group of Sulfonated Block Copolymer Membranes for Direct Methanol Fuel Cell Applications — ***Maritza Perez Perez***, *Eduardo Ruiz Colón, David Suleiman*

2:35 Paper 168f: Invited Talk — ***Whitney G. Colella***

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(169) Phase Behavior and Flow of Reservoir Fluids
Monday, Oct 30, 12:30 PM
MCC, 200B

Michael P. Hoepfner, Chair

Sponsored by:
Upstream Engineering and Flow Assurance Forum

12:30 Paper 169a: Efficient and Robust Multiphase Equilibrium Calculations for Compositional Simulation of CO_2 Injection in Low-Temperature Reservoirs — ***Huanquan Pan***, *Michael Connolly, Hamdi Tchelepi*

12:50 Paper 169b: Phase Behavior in Nanoporous Media and Its Impact on Hydrocarbon Recovery — ***Lin Li***, *Siyong Max Zhang, Alice Z. He, Dengen Zhou*

1:10 Paper 169c: Ultra-Small-Angle Scattering Investigation of the Structure and Self-Assembly Mechanism of Asphaltenes in Solvent Mixtures — ***Yuan Yang***, *Wattana Chaisoontornyotin, Michael P. Hoepfner*

1:30 Paper 169d: An Atomistic Investigation of Hydrocarbon Behavior Confined in Kerogen Nanopores — ***Gorakh Pawar***, *Hai Huang*

1:50 Paper 169e: Effect of Temperature Shift Around Critical Point on Liquid Production from Shales — ***Palash Panja***, *Manas Pathak, Milind Deo*

2:10 Paper 169f: Wettability Analysis of Calcite Aged in Brine, Oil, and Smart Water — ***Imran Khan Shaik***, *Prem Bikkina, Jin Song, Sibani L. Biswal, George J. Hirasaki, Clint P. Aichele*

2:30 Paper 169g: Assessment of Non-Linearities on the Transport Properties of Compressible Fluids — ***Yuan-Yun Lin***, *Michael Myers*

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(170) Process Control Applications
Monday, Oct 30, 12:30 PM
MCC, 103D

David H. Gay, Chair
Ankur Kumar, Co-Chair

Sponsored by:
Systems and Process Control

12:30 Paper 170a: Nonlinear Distributed Model Predictive Control of Gas Sweetening Processes — ***Davood Babaei Pourkargar***, *Manjiri Moharir, Wentao Tang, Ali Almansoori, Prodromos Daoutidis*

12:49 Paper 170b: Dynamic Modeling and Explicit Model Predictive Control of Absorption of Hydrogen in a $LaNi_5$ Bed — ***Gerald S. Ogumerem***, *Efstratios N. Pistikopoulos, Iordanis Kesisoglou*

1:08 Paper 170c: Effective Dose Delivery in Plasma Medicine Using a Robust MPC Approach for Mixed Stochastic and Deterministic Uncertainty — ***Ali Mesbah***, *Joel Paulson, Dogan Gidon, David B. Graves*

1:27 Paper 170d: A Model Reduction and Decomposition Approach for Economic MPC of Wastewater Treatment Plants — *An Zhang,* ***Xunyuan Yin***, *Jing Zeng, Jinfeng Liu*

1:46 Paper 170e: Real-Time Energy Management for Electric Arc Furnace Operation — ***Smriti Shyamal***, *Christopher L. E. Swartz*

2:05 Paper 170f: Multi-Variable Model Predictive Control to Improve Oil Production for Steam-Assisted Gravity Drainage (SAGD) — ***Sagar N. Purkayastha***, *Ian D. Gates, Milana Trifkovic*

2:24 Paper 170g: Real-Time Adaptive Model Predictive Control Framework of Plasma Process — ***Damdae Park***, *Junmo Koo, Solji Choi, Sangwon Ryu, Gon-Ho Kim, Chonghun Han*

2:43 Paper 170h: Load-Following Control for a 10 MWe Supercritical CO_2 Recompression Brayton Power Cycle — ***Jacob Albright***, *Eric A. Liese, Stephen Zitney, Priyadarshi Mahapatra, Debangsu Bhattacharyya*

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(171) Process Design
Monday, Oct 30, 12:30 PM
MCC, 103C

Ana I. Torres, Chair
Emre Gençer, Co-Chair
Mariano Martin, Co-Chair
Selen Cremaschi, Co-Chair
Michael Baldea, Co-Chair

Sponsored by:
Systems and Process Design

12:30 Paper 171a: Optimization-Based Process Synthesis of Processes with Seasonal and Daily Variability: Application on Concentrating Solar Power Plants with Thermochemical Energy Storage — ***Xinyue Peng***, *Thatcher W. Root, Christos T. Maravelias*

12:49 Paper 171b: Anchor-Tenant Models for the Synthesis of Eco-Industrial Parks Through Carbon-Hydrogen-Oxygen Symbiosis Networks — ***Kevin Topolski***, *Mohamed Noureldin, Mahmoud El-Halwagi*

1:08 Paper 171c: Optimal Renewable Production of Ammonia from Water and Air — *Antonio Sánchez,* ***Mariano Martin***

1:27 Paper 171d: Practical Bounds on Reaction Selectivity — *Lorenz Fleitmann,* ***Jeffrey A. Frumkin***, *Michael F. Doherty*

1:46 Paper 171e: Pattern Recognition in Chemical Process Flowsheets — ***Tong Zhang***, *Nick Sahinidis, Jeffrey J. Siirola*

2:05 Paper 171f: Robust Process Flowsheeting Through Nonsmooth Models and Generalized Derivatives — ***Harry A. J. Watson***, *Matias Vikse, Truls Gundersen, Paul I. Barton*

2:24 Paper 171g: A Tightly Constrained MINLP-Based Formulation for the Identification of Energy-Efficient Distillation Configurations — ***Radhakrishna Tumbalam Gooty***, *Parham Mobed, Mohit Tawarmalani, Rakesh Agrawal*

2:43 Paper 171h: A Superstructure-Based Model for Multistream Heat Exchanger Design Within Flow Sheet Optimization — *Harsha Nagesh Rao,* ***Iftekar A. Karimi***

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(172) Quantitative Approaches to Disease Mechanisms and Therapies II
Monday, Oct 30, 12:30 PM
MCC, 208A

Jennifer Pascal, Chair
Ardemis A. Boghossian, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

12:30 Paper 172a: ERK1/2-Driven Sprouty2 Expression Mediates Resistance to Receptor Tyrosine Kinase-Targeted Therapeutics in Glioblastoma — ***Evan K. Day***, *Matthew J. Lazzara*

12:48 Paper 172b: Single-Cycle Growth Kinetics of Infection by Zika Virus — ***Huicheng Shi***, *John Yin*

1:06 Paper 172c: Dynamic Modeling of Pancreatic Cancer Metabolism to Investigate Optimal Therapeutic Strategies — *Mahua Roy,* ***Stacey D. Finley***

1:24 Paper 172d: Regulation of Amyloidogenesis and Proteolysis in the Beta-Amyloid/Cathepsin B/Cystatin C Network — ***Tyler Perlenfein***, *Jacob Mehlhoff, Regina M. Murphy*

1:42 Paper 172e: Receptor Endocytosis and Cell Memory in Growth Factor Signaling — ***Purushottam Dixit***, *Eugenia Lyashenko, Mario Niepel, Dennis Vitkup*

2:00 Paper 172f: Gut Microbiota-Derived Tryptophan Metabolites Modulate Inflammatory Response in Hepatocytes and Macrophages — ***Smitha Krishnan***, *Yufang Ding, Maria Choi, Nima Saedi, Martin L. Yarmush, Arul Jayaraman, Kyongbum Lee*

2:18 Paper 172g: Spatial-Temporal Distribution of RhoA Controls Vascular Barrier Function — ***Stella Alimperti***, *Alexandros Chremos, Varnica Bajaj, Jeroen Eyckams, Jack F. Douglas, Christopher Chen*

2:36 Paper 172h: Integrated Modeling Framework for Signaling, Transcription and Cell Fate and Their Clinical Significance — ***Alokendra Ghosh***, *Ravi Radhakrishnan*

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(173) Rapid-Fire Session: TED-Sep Separations Division
Monday, Oct 30, 12:30 PM
MCC, M100G

John Pellegrino, Chair
Paul Scovazzo, Co-Chair

Sponsored by: Separations Division

12:30 Introductory Remarks

12:40 Paper 401m: Role of Electrokinetics in Glomerular Capillary Filtration: Toward an Artificial Kidney — ***A. Nastasia Allred***, *Samantha Blanton, J. Robby Sanders, Pedro E. Arce*

12:46 Paper 173b: Patterning Various Commercial Nanofiltration and Reverse-Osmosis Membranes — ***Steven T. Weinman***, *Eric Fierce, Scott M. Husson*

12:52 Paper 173c: Preparation of ZIF-8 Membranes Supported on Polymer Hollow Fibers Using Microwave-Assisted Seeding and Secondary Growth Method — ***Moon Joo Lee***, *Mohamad Hamid, Jongmyeong Lee, Ju Sung Kim, Young Moo Lee, Hae-Kwon Jeong*

12:58 Paper 173d: A Zeolitic Imidazolate Framework (ZIF-8) Film for H_2/CO_2 Separation — ***Eunhee Jang***, *Jungkyu Choi*

1:04 Q&A Period 1

1:10 Paper 173e: Scale-Up of Electrochemical Carbon Dioxide Separation Using Membrane Electrode Assemblies — ***Nicholas R. Schwartz***, *Philip Cox, Jason Harrington, Kayla O'Neill*

1:16 Paper 173f: Iron/Palladium Nanoparticle-Functionalized Membrane for Chlorinated Contaminates Treatment — ***Hongyi Wan***, *Nicolas Briot, Anthony Saad, Lindell Ormsbee, Dibakar Bhattacharyya*

1:22 Paper 173g: In-Situ Growth of MOF Membranes Assisted by Electro-Deposition — *Sheng Zhou,* ***Yanying Wei***, *Haihui Wang*

1:28 Paper 173h: Pd/Ta Composite Metallic Membranes for High-Purity Hydrogen Separation: Permeability and Durability — ***Young Suk Jo***

1:34 Q&A Period 2

1:40 Paper 173i: Fabrication and Characterization of Silicalite Membranes Subject to Knudsen and Surface-Diffusion Transportation Regimes — *David Carter, Boguslaw Kruczek,* ***F. Handan Tezel***

1:46 Paper 173j: Effects of Cyanuric Chloride and Its Derivatives on Gas Separation Properties of Polyurethane Membranes — ***Ahmad Arabi Shamsabadi***, *Morteza Sadeghi, Mohammad Dinari, Anahita Ronasi, Masoud Soroush*

1:52 Paper 173k: The Growth of Glycidyl Methacrylate on Ultrafiltration Membrane: Spatial Control on Surface-Initiated AGET-ATRP with Chain End Potential Functionalities — ***Arijit Sengupta***, *Blaine Carter, Xianghong Qian, Ranil Wickramasinghe*

1:58 Paper 173l: Carbon Molecular Sieves for Binary Permeation of N_2/CH_4 and CO_2/CH_4 *Gas Pairs* — ***Shaihroz Khan***

2:04 Q&A Period 3

2:10 Concluding Remarks

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(174) Reaction Path Analysis I
Monday, Oct 30, 12:30 PM
MCC, L100E

Michael T. Klein, Chair
Preetinder S. Virk, Co-Chair
Amrit Jalan, Co-Chair
Andrew J. Adamczyk, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

12:30 Paper 174a: A Graph-Theoretic Moiety Hypothesis for Olefin Yields from High-Severity Pyrolyses of C6 to C12 Cyclo-Alkanes — ***Preetinder S. Virk***

12:52 Paper 174b: Novel Copper (II) Oxide Nanoleaf Catalyst for the Hydrogen Peroxide-Assisted Oxidation of Glycerol to Dicarboxylic Acids: A Combined Theoretical and Experimental Study — ***Quang Thang Trinh***, *Prince N. Amaniampong, Jithin John Varghese, Francois Jerome, Samir H. Mushrif*

1:14 Paper 174c: Kinetics of Cellulose Fragmentation by Pulse-Heated Analysis of Solid Reactions (PHASR) — ***Saurabh Maduskar***, *Paul J. Dauenhauer*

1:36 Paper 174d: Elucidating and Correcting the Unreliability of Continuum Solvation Methods When Modeling Homogeneous Reaction Mechanisms — ***Yasemin Basdogan***, *John A. Keith*

1:58 Paper 174e: Kinetic Modeling of the Production of Green Diesel via Hydroprocessing — ***Pratyush Agarwal***, *Michael T. Klein*

2:20 Paper 174f: Carbohydrate Conformational Cartography — ***Heather Mayes***, *Justin Huber, Samantha Schwartz, Stephen Vicchio*

2:42 Paper 174g: Mechanism Development for the Generation of Furfural in Xylose Pyrolysis — ***Charles J. McGill***, *Phillip R. Westmoreland*

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(175) Refinery Distillation
Monday, Oct 30, 12:30 PM
MCC, 200A

Andrew W. Sloley, Chair
Paul M. Mathias, Co-Chair

Sponsored by: Fuels and Petrochemicals Division

12:30 Introductory Remarks

12:33 Paper 175a: A Framework for Optimization-Based Design of Heat-Integrated Crude Oil Distillation Units Using a Surrogate Model and Support Vector Machine — ***Dauda Ibrahim***, *Megan Jobson, Jie Li, Gonzalo Guillén-Gosálbez*

12:54 Paper 175b: Optimization -Based Design of Energy-Efficient Crude Oil Distillation Systems with Pre-Separation Units — ***Minerva Ledezma-Martínez***, *Megan Jobson, Robin Smith*

1:15 Paper 175c: Vacuum Distillation: Slop Wax Disposition — ***Andrew W. Sloley***

1:36 Paper 175d: Acid Regenerator Optimization for Increased Unit Throughput — ***Kayla Erickson***

1:57 Paper 175e: Vacuum Distillation: Fractionating Wash Zones — ***Andrew W. Sloley***

2:18 Paper 175f Advances in Salt Point Management Practices: Mitigating Overhead Corrosion with Big Data — ***Collin Cross***

2:39 Paper 175g: Fouling Modelling for Crude Oil Heat Exchanger Networks — ***José Loyola-Fuentes***, *Robin Smith, Megan Jobson*

3:00 Concluding Remarks

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(176) Solve This! Fundamental Approach to Problem Solving in Industrial Processes I (Invited Talks)
Monday, Oct 30, 12:30 PM
MCC, 101I

Zdravko Stefanov, Chair
Paul Chauvel, Jr., Co-Chair
Eldad Herceg, Co-Chair
Dana A. Livingston, Co-Chair

Sponsored by: Young Professionals Committee (YPC)

12:30 Paper 176a: Solve this! Fundamental Approach to Problem Solving in Industrial Processes I (Invited Talks) — ***Zdravko Stefanov, Paul Chauvel, Jr., Eldad Herceg, Dana A. Livingston***

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(177) Synthesis and Application of Porous Materials II: Application
Monday, Oct 30, 12:30 PM
MCC, 209A/B

Sunho Choi, Chair
Satish Nune, Co-Chair
Sandeep Kumar, Co-Chair

Sponsored by: Inorganic Materials

12:30 Paper 177a: Tuning External Surface and Textural Properties of Unit-Cell Thick-Pillared MFI and Pillared MWW Zeolites by Atomic Layer Deposition and Its Consequence on Catalytic Reactions — ***Dongxia Liu***, *Junyan Zhang*

12:52 Paper 177b: Mesoporous TiO_2 to TiO_2-Cellulose Composite and Its Derivatives for Environmental Remediation — *Jinju Zhang, Lei Li, Yanxiang Li, Lixia Cao,* ***Chuanfang Yang***

1:14 Paper 177c: Reliable Fabrication and Surface Modification of Beta Zeolite Membrane for Pervaporation of n-Butanol/Water Mixtures — ***Yun Li***, *Honghong Xu, Tao Chen, Xiufeng Liu, Baoquan Zhang**

1:36 Paper 177d: Investigation of Factors That Induce Cristobalite Formation During Titanosilicate Synthesis and Their Potential Impact on Heterogeneous Catalysis — ***Ayomi S. Perera***, *Haiyue Yu, Jeremy Cockcroft, Panagiotis Trogadas, Marc-Olivier Coppens*

1:58 Paper 177e: Novel Methods to Synthesize ZSM-11 as an Efficient Catalyst for Methanol-to-Hydrocarbon Reactions — ***Yufeng Shen***, *Thuy T. Le, Jeffrey D. Rimer*

2:20 Paper 177f: Preparation of Novel Al-MFI/Fe-MFI Core-Shell Catalysts and Their Catalytic Application for CH_4 Conversion — ***Toshiyuki Yokoi***, *Yoshihiko Kimura, Takaya Kimura, Yusuke Kunitake, Atsushi Muramatsu*

2:42 Paper 177g: An Optimized Procedure for Selective Removal of EFAl (Extra Framework Aluminum) in Y Zeolites — ***Balasubramanian Vaithilingam***, *Gnana Pragasam Singaravel, Abdul Majed Al Katheeri, Stephane M., Mikael Berthod*

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(178) The Food-Energy-Water Nexus
Monday, Oct 30, 12:30 PM
MCC, 102A

Vikas Khanna, Chair
Fengqi You, Co-Chair
Yuan Yao, Co-Chair
Ashley M. Pennington, Co-Chair

Sponsored by: General

12:30 Paper 178a: Invited Talk — ***Urmila M. Diwekar***

12:50 Paper 178b: Meeting Challenges in a Land-Constrained Solar Economy: Co-Production of Energy and Food Using Photovoltaic Systems over Farmland — ***Caleb Miskin***, *E mre Gençer, Xingshu Sun, M. Ryyan Khan, Yiru Li, M. Ashraf Alam, Peter Bermel, Rakesh Agrawal*

1:10 Paper 178c: Embodied Phosphorus in Interstate U.S. Food Transfers: Sustainability Implications for Food-Energy-Water Nexus — ***Nemi Vora***, *Vikas Khanna*

1:30 Paper 178d: Comparing BECCS and DAC for Climate Change Mitigation: The Water-Land-Energy Nexus — ***Habiba A. Daggash***, *Mathilde Fajardy, Niall Mac Dowell*

1:50 Paper 178e: Food Manufacturing: The Shift from Centralised to Distributed Production — *Liliana Angeles-Martinez,* ***Constantinos Theodoropoulos***, *Estefania Lopez-Quiroga, Peter J. Fryer, Serafim Bakalis*

2:10 Paper 178f: Understanding Biomass Value Chains and the Environment-Food-Energy-Water Nexus Through Whole-Systems Analysis and Optimisation — ***Sheila Samsatli***

2:30 Paper 178g: Innovative Approaches to Achieving FEW Nexus Goals That Can Influence Near-Term & Long-Term Decision Making — ***Serpil Guran***

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(179) Thermodynamic and Transport Properties Under Pressure
Monday, Oct 30, 12:30 PM
MCC, M100C

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

Sponsored by: High Pressure

12:30 Paper 179a: Solubility and Phase Equilibria for Optimizing the Processing of Cannabinoids and Terpenes in Cannabis and Hemp Extractions — ***Jerry W. King***

12:50 Paper 179b: Measurement and Modeling of Vinyl Fluoride Solubility in Aqueous Lithium Bis(trifluoromethylsulfonyl)imide Solutions — ***David L. Minnick***, *William J. R. Gilbert, Alejandra M. Rocha, Mark B. Shiflett*

1:10 Paper 179c: Heat and Momentum Transport Properties of CO_2-Expanded Liquids (CXLs): n-Hexane, n-Decane, and n-Tetradecane — *Kourosh Kian,* ***Aaron M. Scurto***

1:30 Paper 179d: Van Der Waals Phenomenological Transport Equation of State for Dense Viscosities of the Ultra-Deep Petroleum Reservoirs in the Gulf of Mexico — ***Akanni S. Lawal***

1:50 Paper 179e: Viscosity Models for Hydrocarbons at High Pressure: A State-of-the-Art Review — ***Isaac Gamwo***, *Hseen O. Baled, Mark A. McHugh, Robert M. Enick*

2:10 Paper 179f: Quantification of Uncertainties in Experimental Liquid Density and Viscosity at HTHP Conditions by Using the Corresponding States Law as Arbitrator — ***Akanni S. Lawal***

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(180) Tools for Product Design
Monday, Oct 30, 12:30 PM
MCC, 102B

Kevin G. Joback, Chair
Honglin Qu, Co-Chair

Sponsored by: Product Design

12:30 Introductory Remarks

12:33 Paper 180a: From Atom Groups to Molecules and Mixtures/ Formulations: A Comprehensive Design Methodology with Generalized Disjunctive Programming — *Suela Jonuzaj, Aparana Gupta,* ***Claire S. Adjiman***

12:56 Paper 180b: A Novel Computer-Aided Model-Based Tool for Chemical Product Design — ***Sawitree Kalakul***, *Mario Richard Eden, Rafiqul Gani*

1:19 Paper 180c Antibiotics Molecular Design Using Artificial Bee Colony Optimization — ***Shweta Mapari***, *Matthew Hartenstein, Rex Gaumer, Kyle Camarda*

1:42 Paper 180d: An Integrated Methodology for Chemical Product Design: Application to Hair-and Skin-Care Emulsions — *Javier Arrieta-Escobar, Fernando P. Bernardo,* ***Alvaro Orjuela***, *Mauricio Camargo, Laure Morel*

2:05 Paper 180e: Computer-Aided Modeling for Tailor-Made Design of Surrogate Fuels — ***Lei Zhang***, *Sawitree Kalakul, Linlin Liu, Nimir O. Elbashir, Jian Du, Rafiqul Gani*

2:28 Paper 180f: Product Design: A Systematic Pricing Framework for Maximizing Company Profits — *Yuk C. Chan,* ***Ka Y. Fung***, *Ka Ming Ng*

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(181) Undergraduate Engineering Education of Ethics
Monday, Oct 30, 12:30 PM
MCC, L100G

Deborah Grubbe, Chair
Scott Love, Co-Chair

Sponsored by: Professional Development

12:30 Introductory Remarks

12:40 Paper 181a: Road Map for Embedding Ethics into ChE Undergraduate Curricula — ***Deborah Grubbe***

1:02 Paper 181b: Views on Ethics in Undergraduate Education — ***Dorothy W. Skaf***

1:24 Paper 181c: Ethical Reasoning in the Engineering Curriculum — ***Raffaella Ocone***

1:46 Paper 181d: Engineering Ethics & Educations — ***Spyros Tseregounis***

2:08 Panel Discussion Featuring: Dorothy Skaf, Raffaella Ocone, and Spyros Tseregounis

2:53 Concluding Remarks

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(182) Soft Matter Electrokinetics: Particles, Drops, and Bubbles
Monday, Oct 30, 1:15 PM
Hilton, Marquette IV/V/VI/VII

Stuart J. Williams, Chair
Christopher L. Wirth, Co-Chair

Sponsored by: 2017 Annual Meeting of the AES Electrophoresis Society

1:15 Paper 182a: Understanding the Role of Electrokinetics-Hydrodynamics in Electrical Field–Based Soil Remediation — ***Oluwatosin Owoseni***, *Pedro E. Arce, Yung-Way Liu*

1:30 Paper 182b: Electrohydrodynamics of a Viscous Drop — ***Yuan-Nan Young***, *Herve Nganguia, On Shun Pak*

1:45 Paper 182c: Electro-Hydrodynamic Behavior of Soft Liquid Metal Plugs Under Low Voltages — ***Ishan D. Joshipura***, *Yash Patil, Michael D. Dickey*

2:00 Paper 182d: A Model for Electrokinetic Flow with Deformable Interfaces — ***Michael Booty***, *Rui Cao, Manman Ma, Michael Siegel*

2:15 Paper 182e: Monodispersed Droplet Generation Using AC Electric Field — ***Zehao Pan***, *Yongfan Men, Satyajyoti Senapati, Hsueh -Chia Chang*

2:30 Paper 182f: Crater Formation on Electrodes During Charge Transfer with Aqueous Droplets or Solid Particles — ***Eric S. Elton***, *Ethan R. Rosenberg, William D. Ristenpart*

2:45 Paper 182g: The Electric Field in Water Between Parallel Electrodes: A Sinusoidal Applied Potential Can Yield a Non-Zero, Long-Range Steady Field — ***Seyyed Mohammad Hossein Hashemi Amrei***, *William D. Ristenpart, Greg Miller*

3:00 Paper 182h: Moving Past Simple Shapes: Engineered Active Particle Spinners and Motors Powered by AC Electric Fields — ***C. Wyatt Shields IV***, *Koohee Han, Fuduo Ma, Orlin D. Velev*

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(183) Getting Your Research Published (Invited Talks)
Monday, Oct 30, 1:30 PM
MCC, 101A

Steve Smith, Chair

Sponsored by: Publication Committee

1:30 Paper 183a: Panelist: Michael Harold, Editor, AIChE Journal — ***Michael Harold***

1:50 Paper 183b: Panelist: Michael Domach, Editor, Biotechnology Progress — ***Michael M. Domach***

2:10 Paper 183c: Panelist: Samir Mitragotri, Editor, Bioengineering & Translational Medicine — ***Samir Mitragotri***

2:30 Paper 183d: Panelist: Martin Abraham, Editor, Environmental Progress & Sustainable Energy — ***Martin A. Abraham***

TECHNICAL SESSIONS 2017

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2:50 Paper 183e: Panel Discussion Moderated by Jennifer S. Curtis, Dean, College of Engineering, University of California, Davis
— ***Jennifer Sinclair Curtis***

(184) How Engineers Can Work Effectively with In-House Counsel
Monday, Oct 30, 1:45 PM
MCC, M100F

Sponsored by:
Chemical Engineering & the Law Forum

1:45 Paper 184a: Proactively Preparing Experimental Data in Chemical Patent Applications — ***Peter Jay***

(185) Wilson Award Winner
Monday, Oct 30, 3:15 PM
MCC, 200D

Reid Peterson, Chair
Michael Simpson, Co-Chair

Sponsored by:
Nuclear Engineering Division

3:15 Paper 185a: How the Nuclear Engineering Division Influenced My Career — ***Dan P. Lambert***

(186) Interactive Session: Applied Mathematics and Numerical Analysis
Monday, Oct 30, 3:15 PM
MCC, Exhibit Hall B

Martin Guay, Chair
Ashlee N. Ford Versypt, Co-Chair

Sponsored by:
Applied Mathematics and Numerical Analysis

Paper 186a: A Minimalist Model for Rapid Simulation Enabling Optimization of the Uniformity of Multiple Simultaneous Hydraulic Fracture Growth
— ***Cheng Cheng***, *Andrew P. Bunger*

Paper 186b: Development of a Multi-Objective Optimization Tool for Simulation-Based Chemical Process Synthesis and Design Tasks
— ***Kristina Zimmermann***, *Georg Fieg*

Paper 186c: Heat-Exchanger Network Retrofit for Industrial Applications Based on Applied Stage-Wise Model
— *Natchanon Angsutorn*, ***Kitipat Siemanond***, *Rungroj Chuvaree*

Paper 186d: Quenched Periodic Extension for Interpolation Using Radial Basis Functions — ***Rafael G. Henríquez Rivera***, *Ludwig C. Nitsche*

Paper 186e: A Two-Phase Imbibition-Drainage Model for Soils Amended with Biochars — ***Yi Chen***, *Kyriacos Zygourakis*

Paper 186f: The Benefits of Resource Partitioning and Division of Labor in Biofilm-Based Microbial Consortia
— ***Jeffrey J. Heys***, *Ross P. Carlson, Timothy Johnson, Tomas Gedeon*

Paper 186g: Novel Non-Invasive Quantification of Coronary Artery Stenosis — ***Javad Hashemi***, *Shahab Ghafghazi, R. Eric Berson*

Paper 186h: Non-Linear Behavior of Coupled Autocatalytic Reaction Systems — ***P. C. Seshasai***, *S. Pushpavanam, C. Anoop*

Paper 186i: New Method to Compute Local Fluxes and Stresses at the Bubble Surfaces in Multiphase Flow Simulation — ***M. Helal Uddin***, *Charles Coronella*

Paper 186j: Theoretical Analysis and Process Design for Dual-Impinging Jet Cooling Crystallization — ***Mo Jiang***, *J. Carl Pirkle Jr., Richard D. Braatz*

Paper 186k: A Simple Numerical Approach for Solving Population Balance Equations — ***L. Ivano Costa***

Paper 186l: Analytical Solution of the Period of Belousov-Zhabotinsky Reaction Using a Feedback Mechanism
— ***Chi Zhai***, *Wei Sun, Ahmet Palazoglu*

Paper 186m: Physically Based Dynamic Modeling for Predictive Simulation of a Net-Zero Home
— *Alan Uy*, ***Raymond Adomaitis***

Paper 186n: Comparison of Various Techniques for Solving Complex Chemical Equilibrium Problems
— ***Mordechai Shacham***, *Neima Brauner*

(187) Interactive Session: Data and Information Systems
Monday, Oct 30, 3:15 PM
MCC, Exhibit Hall B

Donald J. Chmielewski, Chair
Matthew Realff, Co-Chair

Sponsored by:
Data and Information Systems

Paper 187a: Development and Proving of an Information System
— ***Holger Mayer***, *Georg Fieg*

Paper 187b: Evaluating Hospital Performance Using Process Systems Engineering Tools — ***Jangwon Lee***, *Ravi Chinta, Q. Peter He*

Paper 187c: DeepMetabolism: A Deep Learning Algorithm to Predict Phenotype from Genome Sequencing
— ***Weihua Guo***, *You Xu, Xueyang Feng*

Paper 187d: Multiscale Dynamics System Identification of Time Series of Riser Reactor Temperature in FCC Process Based on Hilbert-Huang Transform — ***Daofan Cao***, *Yingya Wu, Xingying Lan, Jinsen Gao, Chunming Xu*

Paper 187e: Next-Generation Process Monitoring for IoT-Enabled Smart Manufacturing — ***Q. Peter He***, *Jin Wang*

Paper 187f: Reaction Identification and Parameter Estimation from Chemical Process Data — ***Zachary Wilson***, *Nick Sahinidis*

Paper 187g: Plant-Wide Visualization for Situation Awareness Using Ising Model-Based Clustering of Vanishing Correlations — ***Masanao Natsumeda***

Paper 187h: Process Monitoring Using a PCA-Based Exponentially Weighted Generalized Likelihood Ratio Chart
— *M. Ziyan Sheriff*, ***Chiranjivi Botre***, *Majdi Mansouri, M. Nazmul Karim, Hazem Nounou, Mohamed Nounou*

Paper 187i: An Inverse-Model-Based Methodology for Real-Time Fault Diagnosis in Non-Square Multivariate Dynamic Systems — ***Liwen Chen***, *Qiang Xu*

Paper 187j: Root-Cause Diagnosis of Process Fault Using Modified Convergent Cross-Mapping and Bayesian Network — ***Feifan Cheng***, *Jinsong Zhao*

Paper 187k: Time-Frequency Analysis of Pupillary Fluctuations to Monitor Control Room Operators During Plant Abnormalities
— ***Punitkumar Bhavsar***, *Babji Srinivasan*, ***Rajagopalan Srinivasan***

(188) Interactive Session: Systems and Process Control
Monday, Oct 30, 3:15 PM
MCC, Exhibit Hall B

Juergen Hahn, Chair
Mona Bavarian, Co-Chair

Sponsored by:
Systems and Process Control

Paper 188a: Model Reduction of Underdamped Modes for the SIMC Tuning of PI Controllers — ***Jietae Lee***, *Yongjeh Lee, Dae Ryook Yang, Thomas F. Edgar*

Paper 188b: Fractional Order Plus Time Delay Model Extending the First Order Plus Time Delay Model
— ***Yongjeh Lee***, *Dae Ryook Yang, Jietae Lee, Thomas F. Edgar*

Paper 188c: Development of Biomimetic Approaches for Intelligent Control System Design, Monitoring and Optimization of Advanced Energy Systems — *Temitayo Bankole, Gaurav V. Mirlekar, Ghassan Al-Sinbol, Berhane Gebreslassie, Fernando V. Lima, Mario Perhinschi, Urmila M. Diwekar, Richard Turton*, ***Debangsu Bhattacharyya***

Paper 188d: Non-Intrusive Appliance Load Monitoring Algorithm to Detect Simultaneous State Changes of Electrical Appliances
— ***Nikita Patel***, *Babji Srinivasan*, ***Rajagopalan Srinivasan***

Paper 188e: Controller Design for CSTR Process Output Using a Combination of GA, PSO, Fuzzy and PID Algorithms for Quick Rejection of Process Disturbances
— ***Shounak Datta***, *Mario Richard Eden*

Paper 188f: Sparse Controlled Variable Selection for Self-Optimizing Control
— ***Xiao Yang***, *Nan Zhang, Robin Smith*

Paper 188h: Strategies for Minimum-Variance ALS Estimation of Noise Covariance Matrices
— ***Travis J. Arnold***, *James B. Rawlings*

Paper 188i: Stability Analysis of Model Predictive Control Using Piecewise Affine Models Under Unstructured Uncertainty
— ***Panagiotis Petsagkourakis***, *William P. Heath, Constantinos Theodoropoulos*

Paper 188j: Robust Economic Linear Optimal Control — ***Jin Zhang***, *Donald J. Chmielewski*

Paper 188k: Optimal Operation of Heat Exchanger Networks Through Heat Duty Redistribution Using Energy Flow Graphs — ***Sujit S. Jogwar***

Paper 188l: Steady-State Real-Time Optimization of a Reactor-Separator-Recycle Process — ***Nitin Kaistha***, *Vivek Kumar*

Paper 188m: A Multi-Parametric Bi-Level Optimization Strategy for Hierarchical Model Predictive Control
— ***Styliani Avraamidou***, *Nikolaos A. Diangelakis, Efstratios N. Pistikopoulos*

Paper 188n: Computation of Terminal Constraints for Large-Scale NMPC
— ***Devin Griffith***, *Lorenz T. Biegler*

Paper 188o: Approximate Dynamic Programming for Nonlinear Process Control Under Uncertainty — ***Yu Yang***

Paper 188p: A Biologically Inspired Optimal Control Framework: Application to the Hybrid Performance (HyPer) System — ***Gaurav V. Mirlekar***, *Paolo Pezzini, Kenneth M. Bryden, David Tucker, Fernando V. Lima*

Paper 188q: CFD Simulation of Charged Aerosol Combustion Under High Electric Field — ***Yeonpyeong Jo***, ***Soojin Kwon***, *Sungwon Hwang*

Paper 188r: A Case Study on Semi-Batch Endpoint Control
— ***Nishith R. Patel***, *James B. Rawlings*

Paper 188s: Modeling the Effect of Tube Replacement on the Operation of Primary Reformer in Ammonia Plant
— ***Muhamad Fariz Failaka***, *Fildzah Hanifati, Ali Elkamel*

Paper 188t: Identification of Piecewise Autoregressive Exogenous (PWARX) Model Using Efficient Optimization Algorithm — ***Yu Yang***

Paper 188v: Closed-Loop Re-Identification of Multi-Rate System Using N4SID and Zone MPC
— ***ByungJun Park***, *Se-Kyu Oh, Jong Min Lee*

Paper 188w: Data-Driven Modeling and Optimization of an Ethane Steam Cracker — ***Burcu Beykal***, *Onur Onel, Efstratios N. Pistikopoulos*

Paper 188x: Dual-Rate Approach for Data-Driven Modeling and Prediction of Behavior of Processes with Variations in Sampling Frequencies
— ***Jingwei Gan***, *Satish J. Parulekar, Ali Cinar*

Paper 188y: Nonlinear System Identification and Dynamic Real-Time Optimization of Postcombustion CO_2 Capture Processes for Cycling Applications — ***Rebecca Kim***, *Fernando V. Lima*

Paper 188z: Sparse Kernel Filtering Algorithms for Online Glucose Prediction in T1D — ***Xia Yu***, *Mudassir Rashid, Jianyuan Feng, Nicole Frantz, Iman Hajizadeh, Sediqeh Samadi, Mert Sevil, Caterina Lazaro, Zacharie Maloney, Elizabeth Littlejohn, Laurie Quinn, Ali Cinar*

Paper 188aa: Uniting Lyapunov-Based MPC with Closed-Loop Subspace Identification — ***Masoud Kheradmandi***, *Prashant Mhaskar*

(189) Interactive Session: Systems and Process Design
Monday, Oct 30, 3:15 PM
MCC, Exhibit Hall B

Thomas A. Adams II, Chair
Monica Zanfir, Co-Chair

Sponsored by:
Systems and Process Design

Paper 246l: MOSAIC: Parallel Computing, Multi-objective Optimization Applicationsl
— ***Bridgette Befort***, *Kyle Camarda*

Paper 246e: A Mindset Change from Batch to Continuous Pharmaceutical Crystallization Process Control: The Residence Time-Based Feedback Control — ***Qinglin Su***, *Zoltan K. Nagy*

Paper 189c: Computer-Aided Analysis About the Flow Channel Structure Effect on the Vanadium Redox Battery
— ***Yeong Jae Jeon***

Paper 189d: Optimization of Cryogenic Carbon Dioxide Capture and LNG Processes by Shaft Work Minimization and Mathematical Programming
— ***Orakotch Padungwatanaroj***, ***Kitipat Siemanond***

Paper 189e: Multi-Period Heat Exchanger Network Retrofit Under Fouling Effects — ***Kitipat Siemanond***, ***Supapol Rangfak***

Paper 189f: Reputation-Based Market on the Blockchain Platform: An Emission-Trading Application
— ***Khamila N. Khaqqi***, ***Kunn Hadinoto***, ***Jia Wei Chew***, *Markus Kraft*

Paper 189g: Sustainable CO_2 Utilization in DMC Production
— ***Bjartur Jacobsen***, ***Frederikke Zilstorff***

Paper 189h: Systematic Process Design of a Styrene Production Plant Using a Hierarchical 12-Task Procedure: Waste Stream Utilization for Improved Sustainability
— ***Mathias Johansen***, ***Thomas G. Andersen***, ***Mads G. Andersen***, *Nipun Garg*

Paper 189i: Sustainable Production of Dimethyl Carbonate and Ethylene Glycol via a Systematic Process Design Framework — ***Abhimanyu Pudi***, ***Bhaskar B. Koyyalamudi***, ***Pablo D. Martínez***, *Maria-Ona Bertran, Spardha Jhamb*

Paper 189j: Optimal Use of Water for Hydraulic Fracking of Gas Shale Production — ***Dulce Celeste López-Díaz***, *Luis Fernando Lira-Barragan, Medardo Serna-González, José María Ponce-Ortega*

Paper 246b: The Design of Beta Amino Acid Fragments to Inhibit the Aggregation of Alpha Synuclein
— ***Rex Gaumer***, *Matthew Hartenstein, Kyle V. Camarda*

Paper 246c: Sustainable and Efficient CO_2 Utilization: Production of Dimethyl Carbonate by an Indirect Route Using Ethylene Oxide and Methanol
— ***Adem R. N. Aouichaoui***, ***Anders J. S. Olsen***, ***Kevin C. Feldmann***, *Spardha Jhamb*

Paper 246g: Biochemical Process Design: The Sustainable Production of Biobutanol from Wheat Straw Using *Clostridium acetobutylicum*
— ***Andreas Norgreen***, ***Caroline Norgreen***, ***Christina Etler***, *Olivia Ana Perederic*

Paper 189n: A Systematic Process Design for Sustainable Dimethyl Carbonate Production Through Carbon Dioxide Utilization — ***Jeska Naujoks***, ***Shwetha Meena Sakthi Nallasivam***, ***Niranchana Venkatesh***, *Spardha Jhamb*

Paper 189o: Evaluation of Carbon Monetization in Power Systems for Flaring Mitigation — ***Javier Tovar-Facio***, *Luis Fabian Fuentes-Cortes, José María Ponce-Ortega*

Paper 189p: A Study on Maximizing the Energy Utilization of Process Operation by Integrating Multiple Energy Sources — ***Jun-Hyung Ryu***, *Donghyun Lee, In-Beum Lee*

Paper 189q: Development of Reaction Mechanism and Kinetics for the Production of Butadiene Through Oxidative Dehydrogenation of Alkane or Alkene — ***Junghoon Kim***, *Sungwon Hwang*

Paper 189r: Multiobjective Tabu Search for Plant Design Models
— *Austin Keller, Kyle V. Camarda*, ***Faiz Mandani***

Paper 189s: Stochastic Optimization to Reduce Cost of Energy for Parabolic Trough Solar Power Plant
— ***Urmila M. Diwekar***, *Dev Parikh*

Paper 246d: Superstructure Formulation and Optimization of a Methane-Based Chemical Refinery for Co-Producing Olefins and Aromatics
— ***Zhihong Yuan***

Paper 246j: CFD Modeling of Piston-Type Direct Work Exchangers
— ***Aida Amini Rankouhi***, *Yinlun Huang*

Paper 189v: An Optimization-Based Design and Analysis of a Biomass-Derived Hydrogen Energy System
— ***Seolhee Cho***, *Minji Lee, Jiyong Kim*

Paper 189w: Multi-Objective Optimization of Heat Exchanger Networks Based on Economic and System Reliability by NSGA-I
— ***Wu Xiao***, *Junfeng Lv, Xiaobin Jiang, Gaohong He, Debalina Sengupta, Mahmoud El-Halwagi*

Paper 246k: Simultaneous Process Synthesis and Heat Integration Using a Single Superstructure
— ***Salih E. Demirel***, *Jianping Li, M. M. Faruque Hasan*

Paper 246f: Computational Evaluation of the Performance of Three Treatment Chamber Designs for Electric-Field-Assisted Microbial Inactivation Process
— ***Hassan Masood***, *Patrick J. Cullen, Francisco J. Trujillo*

Paper 246a: A Simultaneous Utility and Area Targeting Model for Integrated Process and Heat Exchanger Network Synthesis — ***Lingxun Kong***, *Christos T. Maravelias*

Paper 246i: A Superstructure-Based Assessment Framework for Downstream Bio-Separation — ***Wenzhao (Tony) Wu***, *Kirti Maheshkumar Yenkie, Christos T. Maravelias*

Paper 189ab: An Efficient Approach to Bounding Multistage Stochastic Programs Using Sample Average Approximation — ***Katie Martin***, *Brianna Christian, Selen Cremaschi*

Paper 246h: Probabilistic Process Design Under Uncertainty via Dynamic Optimization — ***Calvin Tsay***, *Richard Pattison, Michael Baldea*

Paper 189ad: A New Proactive Methodology for Robust Berth Planning of Container Vessels — ***Jialin Xu***, *Prathamesh A. Purohit, Qiang Xu*

Paper 189ae: Optimal Sampling Locations to Reduce Uncertainty in Contamination Extent in Water Distribution Systems
— ***Jose S. Rodriguez***, *Michael Bynum, Katherine A. Klise, Carl Laird, Terranna Haxton, David Hart, Regan Murray*

(190) Interactive Session: Systems and Process Operations
Monday, Oct 30, 3:15 PM
MCC, Exhibit Hall B

Fengqi You, Chair
Chrysanthos E. Gounaris, Co-Chair

Sponsored by:
Computers in Operations and Information Processing

Paper 190a: A Multi-Stakeholder Approach for the Optimal Planning and Integration of the Supply Chain of Fuels Involving CO_2 Capture — ***Aurora de Fátima Sánchez-Bautista***, *Luis Fabian Fuentes-Cortes, José Ezequiel Santibañez Aguilar, J. Betzabe González-Campos, José María Ponce-Ortega*

Paper 190b: A New Continuous-Time Model for Short-Term Scheduling of Multipurpose Batch Plants Using Non-Uniform Time Grid — ***Érica Victor***, *Valeria Murata, Sergio Neiro*

Paper 190c: Optimal Control Structure Design for Cyber-Physical Systems — ***Temitayo Bankole***, *Paolo Pezzini, Nor Farida, Kenneth M. Bryden, David Tucker, Debangsu Bhattacharyya*

Paper 190d: A Study for Integration of Procurement Planning and Short-Term Scheduling in Petroleum Refineries — ***Jialin Xu***, *Qiang Xu*

Paper 190e: Hybrid Modeling of Bioreactor Systems Using First Principles and Deep Neural Networks with Constraints of Validity Domain for Optimization of Feeding Strategy — ***Jaehan Bae***, *Hyeji Lee, Dong Hwi Jeong, Jong Hwan Shin, Jong Min Lee*

Paper 190f: Dynamic Modeling and Control of a Natural Gas Combined Cycle (NGCC) Power Plant Integrated with CO_2 Capture — ***Yifan Wang***, *Debangsu Bhattacharyya, Richard Turton*

Paper 190g: Exposure Reconstruction of Multiple Chemicals from Human Biomonitoring Data Using Markov Chain and Differential Evolution Monte Carlo — *Dimosthenis Sarigiannis, Evangelos Handakas, Alberto Gotti,* ***Spyros Karakitsios***

Paper 190h: Combined Dynamic Simulation and Scheduling Optimization of Shutdown Procedures of Ethylene Plants — ***Jian Zhang***, *Qiang Xu, Thomas Ho*

Paper 190k: Single- and Multi-Objective Optimizations Using Parallelized Process Simulators — ***Trevor Rice***, *Aaron Herrick, Mingder Lu*

Paper 190l: Term Elimination and Optimal Experiments for Model Reduction — ***Brian Baillie***, *George M. Bollas*

Paper 190n: Scalable Modeling and Solution of Stochastic Multiobjective Optimization Problems — *Yankai Cao, Luis Fabian Fuentes-Cortes,* ***Victor M. Zavala***

Paper 190o: Optimal Refinery Crude Scheduling with Considerations of Crude Mixing Along with the Pipeline Transportation — ***Honglin Qu***, *Qiang Xu*

Paper 190p: Stochastic Optimization of Carbon Dioxide Supply Chain and Utilization Model — ***Narut Suchartsunthorn***, ***Kitipat Siemanond***

Paper 190q: Turnaround ALPS: Making Turnaround Time Shorter — ***Pavel Vacha***, *Richard Dobis, Viktor Popovic*

Paper 190r: Optimal Planning Under Uncertainty for a Supply Chain Focused on Residual Biomass Conversion Using Geographic Information Systems and Mathematical Programming — ***José Ezequiel Santibañez-Aguilar***, *Diego Fabián Lozano-García, Francisco José Lozano, Antonio Flores-Tlacuahuac*

Paper 190s: An Optimization Approach to Ordinary-Fractional Multi-Compartmental Models with Applications to Pharmacokinetics and Optimal Drug Usage — ***Vicente Rico-Ramirez***, *Julio C. Barrera-Martinez, Edgar O. Castrejon-Gonzalez, Edna S. Lopez-Saucedo*

Paper 190t: Bilevel Optimization Strategies to Couple Production of Biotechnological Products with Growth in Cyanobacteria — *Romina Lasry Testa, Claudio Delpino, Vanina Estrada,* ***Maria Soledad Diaz***

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(191) Poster Session: Bioengineering
Monday, Oct 30, 3:15 PM
MCC, Exhibit Hall B

Adam Melvin, Chair
Derek Englert, Co-Chair
Ryan Summers, Co-Chair
Seok Hoon Hong, Co-Chair
Rajib Saha, Co-Chair
Nicholas R. Sandoval, Co-Chair

Sponsored by: Bioengineering

■ SYNTHETIC BIOLOGY

Paper 191a: Optogenetic Platform for the "On-Demand" Production of Proteins in Biopharma and Biomedical Applications — ***Everardo González-González***, *Grissel Trujillo-de Santiago, Mario M. Alvarez*

Paper 191b: Considerations for Using Hammerhead-Based Riboswitches in the 5′-UTR to Control Genes in Bacteria — *Wanqi Sun,* ***Ryan M. Summers***

Paper 191c: Strategies for Quorum Sensing Inhibition in *Staphylococcus aureus* — ***Moises Contreras-Ramos***, *James Lichty, Thomas J. Mansell*

Paper 191d: Heterologous Expression of Highly Specific Antimicrobial Peptides in Probiotic *E. coli* — ***Halimatun Zainuddin***, *Thomas J. Mansell*

Paper 191e: Heterologous Reconstitution of the Quorum Sensing System of *Clostridium difficile* in Non-Pathogenic Hosts — ***James Lichty***, *Ashley Iannuzzelli, Thomas J. Mansell*

Paper 191f: Directing the Self-Assembly of Multiple DNA Nanostructures in a Single Reaction — ***Vasiliki Kolliopoulos***, *Carlos E. Castro*

Paper 191g: Engineering Probiotic Bacteria for the Delivery of Antimicrobial Peptides to the Intestines — ***Kathryn Geldart***, *Brittany Forkus, Madeline Forbes, Yiannis N. Kaznessis*

Paper 191h: Fine-Tuning of the Flavonoid Biosynthesis Pathway by Promoter Strategies — ***Jingwen Zhou***

Paper 191i: Treatment of Autosomal Dominant Progressive Hearing Loss by In-Vivo Delivery of Genome Editing Agents — ***Xue Gao***

Paper 191j: Optogenetic Toolkit for Rapid and Reversible Control of Gene Expression in Bacteria — ***Chueh Loo Poh***, *Premkumar Jayaraman*

Paper 191k: The Mammalian LINC Complex Regulates Genome Transcriptional Responses to Substrate Rigidity — *Samer Alam,* ***Qiao Zhang***, *Nripesh Prasad, Yuan Li, Srikar Chamala, Ram Kuchibhotla, Birendra K. C., Varun Aggarwal, Shristi Shrestha, Angela L. Jones, Shawn E. Levy, Kyle Roux, Jeffrey A. Nickerson, Tanmay Lele*

■ BIOCATALYSTS & BIOBASED PRODUCTS

Paper 191l: Engineering of the Yeast Membrane for Increased Biorenewable Chemical Production — ***Kirsten Davis***, *Laura Jarboe, Jeffery Klauda*

Paper 191m: Electricity from Methane by Reversing Methanogenesis Using an Engineered Consortium — ***Thomas K. Wood***

Paper 191n: Reverse Engineering of Short-Chain Fatty Acid Tolerance and Production in *Escherichia coli* — ***Yingxi Chen***, *Erin Boggess, Julie Dickerson, Thomas J. Mansell, Laura Jarboe*

Paper 191o: Kinetics of Silver Cation Diffusion Across an Algal Cell Wall During Silver Nanoparticle Biosynthesis — ***Tsai-Nan Mai***, *Ashiqur Rahman, Shishir V. Kumar, Julia Lin, Si Amar Dahoumane, Clayton S. Jeffryes*

Paper 191p: The Global Regulator IrrE from *Deinococcus radiodurans*–Enhanced *Saccharomyces cerevisiae* Tolerances Toward Furfural — ***Jufang Wang***, *Ping Luo, Hongxin Fu*

Paper 191q: Discovery and Characterization of Novel Bacterial Monomodular Type I Polyketide Synthases — ***Bin Wang***

Paper 191r: Extremophilic Biopolymer-Based Films: Production, Characterization, and Application — ***Jia Wang***, *David R. Salem, Rajesh K. Sani*

Paper 191s: A Platform for Biosynthesis of D-Amino Acids — ***Qiuge Zhang***, *Kechun Zhang*

Paper 191t: Reaction Engineering and Pathway Development for an Enzymatic Route from Furfural to 2,5-Furandicarboxylic Acid (FDCA) — ***Harrison B. Rose***, *Aimee C. Moise, Madison M. Wilber, John M. Robbins, Andreas S. Bommarius*

Paper 191u: Homologous Constitutive Secretory Expression of Halo, Acid and Thermo-Tolerant β-Glucosidase in Marine *Aspergillus niger* — ***Li-Nian Cai***, *Dong-Qiang Lin, Shan-Jing Yao*

Paper 191dp: Understanding Preferential Consumption of Aromatic Compounds in Acinetobacter baylyi ADP1 — ***Stephen Lillington***, *William Bothfeld, Keith E.J. Tyo*

Paper 696h: A Simple One-Step Deposition of Zwitterionic Polymer for Providing Biomaterials' Antifouling Ability Via Aminomalononitrile Polymerization — *Wen-Hsuan Chen, Helmut Thissen,* ***Wei-Bor Tsai***

■ CELL CULTURE ENGINEERING

Paper 191v: Spray Delivery of Organoids to Reconstitute Intestinal Epithelium on Decellularized Native Extracellular Matrix — ***Meryem Pehlivaner***, *Dana Schwartz, Allan Goldstein, Harald Ott, Adam Ekenseair*

Paper 191w: Establishing a Toxicity Threshold for Polymeric Nanoparticles in Pulmonary Cells — ***Jordan A. Hoops,*** *Timothy M. Brenza*

Paper 191x: Construction of Human Bronchial Epithelium Culture Platform for Inhalation Drug Development — *Hsin-Lin Hsieh, Pulak Nath,* ***Jen-Huang Huang***

Paper 191y: New Approaches in Engineering Somatic Embryogenesis in Loblolly Pine Suspension Cultures — ***Elizabeth M. Cummings Bende***, *Rachael J. Messier, Sarah A. Wilson, Susan C. Roberts*

Paper 191z: Using Ultrasound Standing Wave–Incorporated Dynamic Photobioreactor System to Enhance Medium Replacement Efficiency for Concentrated Microalgae Cultivation in Continuous Mode — ***Yu-Hsiang Lee***, *Po-Han Li*

Paper 191aa: Chemically Modified mRNA-Based CRISPR-Cas9 System Improves the Viability of Cryopreserved Mammalian Cells — ***Yong Hu***, *Lei Li, Yin Yu, Haishui Huang, Basak Uygun, Martin Yarmush*

Paper 191ac: Elucidating and Engineering the Role of Arabinogalactan Proteins in Somatic Embryogenesis — ***Elizabeth M. Cummings Bende***, *Marcus P. Lundgren, Kara P. Upton, Susan C. Roberts*

Paper 191ad: A Segregated Kinetic Model for Antibody-Producing Cell Lines — ***Denizhan Yilmaz***, *Satish J. Parulekar, Ali Cinar*

Paper 191ae: Extracellular Production of Soluble Single-Chain Variable Fragment (scFv) Using Recombinant *E. coli* by Precisely Controlled Fed-Batch Culture with DO-stat — ***Jun-ichi Horiuchi,*** *Yoichi Kumada, Huan Li, Yuichiro Sakamoto*

Paper 191ag: Investigating Clostridium carboxidivorans P7 Metabolisms During Syngas Fermentations — ***Ni Wan***, *Ashik Sathish, Le You, Yinjie Tang, Zhiyou Wen*

Paper 191ah: CFD Modeling of Bioreactor Mixing Properties — ***Michael Nelson,*** *Jennifer Pollard*

Paper 191ai: Targeted Protein Therapeutics as Powerful Tools for Understanding and Overcoming Drug Resistance in Cancer — ***Mandana Manzari***

Paper 191aj: Numerical Modelling Strategy for the Scale-Up of Single-Use Bioreactors — ***Justin O'Sullivan***, *Brian Glennon*

Paper 191ak: Challenges in Single-Use Bioprocessing Systems: Evaluating the Cytotoxicity of a Leachate from Plastic Single-Use Bioreactors — *Rhythm R. Shah, Joseph Kitchen, Kyle W. Leonard,* ***Christopher Brazel***

Paper 191al: Reincubation of Heat-Shocked *Pseudomonas aeruginosa* Biofilm — ***Haydar Aljaafari,*** *Eric Nuxoll*

Paper 67d: Retron-Based Targeted Mutagenesis Enabling *in vivo* Continuous Evolution in *E. coli* — ***Xiang Zheng***, *Tianmin Wang, Xin-Hui Xing, Chunbo Lou, Chong Zhang*

■ METABOLIC ENGINEERING

Paper 191am: Multidimensional Controlling Optimization of Total Biosynthesis of Astaxanthin and Other Natural Products — ***Congqiang Zhang,*** *Heng-Phon Too*

Paper 191an: Construction of a Zeaxanthin Biosynthetic Pathway as the Base for Crocin Synthesis in *Saccharomyces cerevisiae* — ***Yunpeng Cui***, *Fangyu Cheng*

Paper 191ao: Membrane Engineering in *Escherichia coli* to Enhance Production of Bio-Fuels and Chemicals — ***Miguel Chavez-Santoscoy***, *Laura Jarboe*

Paper 191ap: Cell-Free Production of Isobutanol — ***Matthew Wong***, *Jian Zha, Mattheos A. G. Koffas, Marlene Belfort, Georges Belfort*

Paper 191aq: Systematic Carbon and Growth Analysis of a Promising Methanotroph Strain — ***Kyle Stone***, *Q. Peter He, Jin Wang*

Paper 191ar: Improved Production of Small-Molecule Compound Through *E. coli* Metabolic System Optimization — ***Ruiquan Qi***

Paper 191as: Zn Recovery from Electroplating Sludge Using Stirred-Tank Bioreactor — ***Suresh Gupta***, *Sanjay Kumar Verma, Anupam Singhal, S. Ramachandran, Shraddha Mishra, Sandeep Poonia, Poonam Singh*

Paper 191at: Blocking Lactic Acid Pathway for Enhanced HA Production in *C. glutamicum* — ***Fangyu Cheng***, *Sijin Luozhong, Huimin Yu, Zhongyao Shen*

Paper 191au: Intensification of Biosynthesizing Tyramine with Engineering Bacteria Expressing L-Tyrosine Decarboxylase by Permeabilization of Cell Membranes — *Weirui Zhao,* ***Sheng Hu***, *Jun Huang, Shangjing Yao, Zhihua Jin, Lehe Mei*

Paper 191av: Two-Step Biocatalytic Reaction Using Whole Cells for Efficient Production of Phenyllactic Acid from l-Phenylalanine — ***Lehe Mei***, *Weirui Zhao, Sheng Hu, Jun Huang, Changjiang Lv, Shangjing Yao*

Paper 191aw: Evaluation of Culture Conditions on the Production of Antimicrobial Compounds Against *Staphylococcus aureus* from *Lactobacillus viridescens* — *Thiago Sidooski, Savio L. Bertoli, Carolina Krebs de Souza, Michele Debiasi Alberton,* ***Lisiane Fernandes de Carvalho***

Paper 191ax: Engineering Gut Microbes to Treat Metabolic Disorders — *Zachary Mays, Josef Bober,* ***Nikhil U. Nair***

Paper 191ay: Engineering a Rubisco-Deletion *Crypthecodinium cohnii* for Increased Growth and Lipid Accumulation — ***Jinjin Diao***

Paper 191az: Systems Analysis and Engineering of Oleaginous Red Yeasts — ***Zongbao Zhao***

Paper 191ba: Elucidation of Aromatic Metabolism Pathways in a Non-Model, Non-Conventional Oleaginous Yeast — ***Allison Yaguchi***, *Alana Robinson, Erin Mihealsick, Mark Blenner*

Paper 191bb: Engineering Metabolic Pathways by Using Standardized DNA Parts — ***Xiaoqiang Ma***, *Hong Liang, Liming Yang, Kang Zhou*

Paper 191bc: Application of 13C Flux Analysis to Determine Impacts of Media Alterations on Industrial CHO Cell Metabolism — ***Allison G. McAtee Pereira***, *Jason Walther, Myles Hollenbach, Jamey D. Young*

Paper 191bd: Use of an *Escherichia coli* Pyruvate-Overproducing Platform Strain to Produce L-Valine — ***Paul A. Adamczyk***, *Shu Pan, Xiaolin Zhang, Jennifer L. Reed*

Paper 191be: Engineering a Novel 3-Methyl-1-Butanol Biosynthetic Pathway in *Escherichia coli* — ***William Black***, *Kosuke Seki, Ana Jenic, Yixi Wang, Han Li*

Paper 191bf: Next Steps in Engineering *E. coli* Erythromycin Production — ***Lei Fang***, *Blaine A. Pfeifer*

Paper 191bg: Photocatalytic Production of a Jet Fuel Precursor Limonene — ***Nanette R. Boyle***

Paper 191bh: Metabolic Engineering of *Clostridium cellulovoran* for n-Butanol Production from Cellulose — ***Teng Bao***, *Jingbo Zhao, Shang-Tian Yang*

Paper 191bi: Metabolism of the Pyrolytic Sugar Levoglucosan and Engineered Pyrolysate Tolerance in *Lactococcus lactis* — ***Samuel Rothstein***, *Thomas J. Mansell*

Paper 191bj: Efficient Energy Utilization in Carbon-Fixing *Moorella thermoacetica* — ***Junyoung O. Park***, *Nian Liu, Kara M. Holinski, Gregory Stephanopoulos*

■ MODELING & DOWNSTREAM PROCESSING

Paper 191bk: Chiral Membranes for Enantiomer Separation — ***Somdatta Bhattacharya***, *John J. Keating, Xing Zhang, Robert J. Linhardt, Georges Belfort*

Paper 191bl: The Introduction and Removal of β-Glucans in a Biological Purification Process: A Case Study — ***Robert Luo***

Paper 191bm: Numerical Evaluation of the Two-Phase Fluid Dynamics in a Bench-Scale Bioreactor Applied to Microalgae Cultivation — *Leonardo Germer, Larissa Thais Pereira, Savio L. Bertoli, Carolina Krebs de Souza,* ***Lisiane Fernandes de Carvalho***, *Leonardo Machado da Rosa*

Paper 191bn: Polysorbate 80 Disposition Following Tangential Flow Filtration — ***Kristine Rafferty***, *Maria Olu Ogunyankin, William Ying, Sudhir Chakravarthi, Smeet Deshmukh, Lori Burton*

Paper 191bo: Development of a Pegylated Protein for Large-Scale Manufacturing — ***Nikhil Peer***, *Amy Lim, Elaine Wilcox*

Paper 191bp: Purification of a Pegylated Protein — ***Elaine Wilcox***, *Nikhil Peer, Amy Lim*

■ PROTEIN SCIENCE & ENGINEERING

Paper 191br: The Role of Bacterial Outer Membrane Vesicles in Establishing an Ecological Niche — *Justin Nice, Shannon Collins,* ***Angela C. Brown***

Paper 191bs: Engineering Glucose Binding Proteins with a Chemo-Enzymatic Tag for Glucose Detection in Exhaled Breath Condensates (EBC) — ***Divya Tankasala***, *Karin Ejendal, Tamara L. Kinzer-Ursem, Jacqueline C. Linnes*

Paper 191bt: Engineering Novel "Designer" Glycopeptides *In Planta* as a Molecular Carrier for Directing the Accumulation of Recombinant Proteins/Enzymes — ***Jianfeng Xu***, *Ningning Zhang, Gregory Phillips, Brett Savary*

Paper 191bu: Protein Detection Using Paper-Based Graphene Ink Biosensors from a Flexographic Proofer — ***Dylan G. Turpeinen***, *Stephanie M. King, Adrienne Minerick, Hiroyuki Fukushima, Warren F. Perger, Julia A. King, Caryn L. Heldt*

Paper 191bv: Engineering of a Protein Probe for Alpha-Synuclein Detection — ***Jason Candreva***, *Edward Chau, Jin Ryoun Kim*

Paper 191bw: Expression of Snake Antivenom Proteins with *B. subtillis* — ***William Estell***, *Claire F. Komives*

Paper 191bx: Expression of Snake Antivenom Peptide Chain in *Pichia pastoris* — ***Israel Juarez***, *Lilley Tran, William Estell, Claire F. Komives*

Paper 191by: Adoptive Transfer of CAR-Engineered T Cells with Surface-Conjugated Synthetic Nanoparticles Containing Small-Molecule Inhibitors for Reversing Intratumoral T Cell Hypofunction — ***Yu Jeong Kim***, *Natnaree Siriwon, Elizabeth Siegler, Xianhui Chen, Yarong Liu, Pin Wang*

Paper 191bz: Computational Analysis of Solid Tumor Oxygenation Facilitated by Polymerized Human Hemoglobins — ***Donald Belcher***, *Uddyalok Banerjee, Christopher Baehr, Andre Palmer*

Paper 191ca: Metabolomics Approach to Understand a 2-Phase Anaerobic Digester System — ***Sachindra T. Cooray***, *Wei Ning Chen*

Paper 191cb: Luminescent Nanoparticles for High-Throughput Microfluidic Droplet Barcoding — *Manibarathi Vaithiyanathan, Khashayar Ramezani Bajgiran, Pragathi Darapaneni, Riad Elkhanoufi, James Dorman,* ***Adam Melvin***

Paper 191cc: Development of NIR-II Nanoparticle Contrast Agents for Photoacoustic Imaging — ***Leon Z. Wang***, *Hoang D. Lu, Melissa R. Fagan, Tristan L. Lim, Bryan J. Kudisch, Yanglu Chen, Andrew Heinmiller, Gregory D. Scholes, Robert K. Prud'homme*

Paper 191cd: Colorimetric Virus Detection Using Gold Nanoparticle Aggregation — ***Xue Mi***, *Stephanie Bean, Eugenia Li Ling Yeo, James Chen Yong Kah, Caryn L. Heldt*

Paper 191ce: Engineering Hepatitis B Viral-Like Particles into Protein Delivery Vehicles — ***Emily Hartzell***, *Heejae Kim, Wilfred Chen*

Paper 191cg: Production of Homogeneous Antibody-Drug Conjugates Using the Nucleotide Binding Site — ***Nur Mustafaoglu***, *Franklin Mejia, Michael Canonico, Tanyel Kiziltepe, Basar Bilgicer*

Paper 191ch: Arduino-Based POC System for the Diagnosis of Viral Diseases Through On-Line Conductivity Measurement — ***Mario M. Alvarez***, *Everardo González-González, Azahel Rivera-Silva, Angel Reyes-Aguilar, Grissel Trujillo-de Santiago, Luis Iglesias-Hernández, Ali Khademhosseini*

Paper 191ci: Design of a Cholesterol-Binding Peptide to Inhibit Bacterial Toxin Activity — *Evan Koufos,* ***Angela C. Brown***

Paper 191cj: A Novel Diagnostic Liposomal Platform, Nanoallergen, for Clinical Evaluation of Epitope Immunogenicity of Peanut Allergen — ***Baksun Kim***, *Peter Deak, Jaeho Shin, Maura Vrabel, Amina Abdul Qayum, Tanyel Kiziltepe, Basar Bilgicer*

Paper 191ck: The Discovery of Enzymatically Depolymerized Heparin Derivatives for the Treatment of Ulcerative Colitis — ***Yang Ji***, *Yi Wang, Yuting Lin, Yishu Yan, Shanshan Du, Xinhui Xing, Yuan Lu, Chong Zhang*

Paper 191cl: Methods for Development and Characterization of DNA Polymerase-Based Bio-Recorders — ***Namita Bhan***, *Alexandra de Paz, Jing Wu, Ted Cybulski, Keith E. J. Tyo*

Paper 191cm: Selection and Affinity Enhancement of Alpha-Synuclein-Specific Single-Domain Antibody Using Experimental and Simulation Techniques — ***Sai Pooja Mahajan***, *Bunyarit Meksiriporn, Dujduan Waraho, Fernando A. Escobedo, Matthew P. DeLisa*

Paper 191cn: Impact of Linker Attachment Site on Structure and Dynamics of Enzymes — ***Siva Dasetty***, *Maxwell Hilbert, Mark Blenner, Sapna Sarupria*

Paper 191co: Building Disulfide Bonds Between Subunits to Improve the Stability of Nitrile Hydratase — ***Song Jiao***, *Jing Zhang, Jie Chen, Huimin Yu*

Paper 191cp: Engineering Bioresponsive Materials from Recombinant Oleosin — ***Chen Gao***

Paper 191cq: Exploiting the PAF Receptor to Target Infectious Diseases in the Lungs — ***Benjamin King***, *Jennifer Fiegel*

Paper 191cr: Interaction of Multiple Drops and Formation of Toroidal-Spiral Particles — ***Paola Leon Plata***, *Ludwig C. Nitsche, Ying Liu*

Paper 191cs: Formation of Aggregates in Perfluorocarbon-Based Oxygen Carriers When Diluted on Plasma Expanders — ***Yissel M. Luengas***, *Alejandra Castilla, Juan C. Briceño Triana, Oscar A. Alvarez*

Paper 191ct: Structural Studies of Protein-Based Nanoparticle Synthesis — ***Brent L. Nannenga***

Paper 191cu: Probing the Influence of Sibling Proteins on Collagen I Fibrillogenesis and Denaturation — ***Matthew T. Bernards***, *Kevin Zurick, Chengyu Jiang*

Paper 191cv: Rational Engineering of Tyrosine Decarboxylase for Efficient Preparation of Tyramine — ***Guochao Xu***, *Haixia Zhu, Ye Ni*

Paper 191cw: Hetero-Assemblies of Beta-Amyloid and Alpha-Synuclein Suggest Correlation Between Alzheimer's and Parkinson's Diseases — ***Jin Ryoun Kim***, *Jason Candreva, Edward Chau*

Paper 191cx: Oxidative Modification of Peptoids Utilizing Bleach and TEMPO as Green Chemistry Catalysts for Protein Therapeutic Applications — ***Jesse Roberts***, *Darla Roberts, Shannon L. Servoss*

Paper 191cy: Resonant Soft X-Ray Scattering of Proteins in Solution — *Dan Ye, Thinh Le, Cheng Wang, Peter H. Zwart, Enrique D. Gomez,* ***Esther W. Gomez***

Paper 191cz: Enhanced Enzyme Activity Through Photoreversible Conformational Changes — ***Yimin Wang***

Paper 191da: Light-Controlled Protein Dynamics Observed with Neutron Spin Echo Measurements — ***Yimin Wang***

Paper 191db: Engineered Bacterial Biosensor to Detect Endocrine Disruptors — ***Ariel Furst***, *Matthew Francis*

Paper 191dn: Maximizing P-Glycoprotein Expression and Transport in the Presence of Therapeutic Compounds — ***Hope Holt***, *Elizabeth Moore, Fransico Gonzalez, Melissa A. Moss*

Paper 191dq: Single-cell Analysis for Identifying an Effective Combination Therapy for Melanoma — ***Yapeng Su***, *Wei Wei, Min Xue, Lidia Robert, Jennifer Tsoi, Thomas Graeber, Raphael Levine, Antoni Ribas, James Heath*

■ SYSTEMS & QUANTITATIVE BIOLOGY

Paper 191dc: Towards Modeling of Methane Recycling Lake Washington Microbial Community — ***Tony Le, Shardhat Daggumati***, *Rajib Saha*

Paper 191dd: Systems Biology Analysis of Natural Biomass Utilization Microbiomes for Biotechnology Applications — ***Joshua Yuan***

Paper 191de: Metabolic Pathway Engineering in Mammalian Cells Through Kinetic Model Optimization — ***Conor O'Brien***, *Andrew Allman, Wei-Shou Hu, Prodromos Daoutidis*

Paper 191df: In-Silico Analysis: A Tool to Suggest Testable Hypotheses — *Shraddha Puntambekar, Dimpal Nyayanit, Apurva Badkas,* ***Chetan J. Gadgil***

Paper 191dg: Comparative Transcriptomics Analysis Pipeline for a Customized CHO Microarray Platform — ***Chun Chen***, *Brian Follstad, Huong Le, Chetan Goudar*

Paper 191dh: An Efficient Brownian Dynamics Approach for Modeling Multivalent Ligand-Receptor Assembly in the Cell Membrane — ***Dipak Barua***

Paper 191di: A Deep-Learning Framework Decodes Coordination of Microbial Metabolism Under Genetic and Environmental Perturbations — ***Tolutola Oyetunde***, *Jeffrey Czajka, Yinjie Tang*

Paper 191dj: Predicting Metabolic Disruptions Due to Heterologous Pathway Expression — ***Sara Amin***, *Venkatesh EndalurGopinarayanan, Nikhil U. Nair, Soha Hassoun*

Paper 191dk: Maximum Entropy Prediction of Distributions for Stochastic Biochemical Reaction Networks with Oscillatory Dynamics — ***Pedro Constantino***, *Yiannis N. Kaznessis*

Paper 191dl: Agent-Based Modeling of a Mammalian Cell Culture Bioreactor with High-Performance Computing to Predict Cell Behavior — ***Robert Jackson***, *Seyed Mostafa Safdarnejad, Elif S. Bayrak, Tony Wang, Radu Georgescu, Myra Coufal, Chetan Goudar, Cenk Undey, Ali Cinar*

(192) Poster Session: Computational Molecular Science and Engineering Forum (CoMSEF)
Monday, Oct 30, 3:15 PM
MCC, Exhibit Hall B

Jim Pfaendtner, Chair
Christina M. Payne, Co-Chair

Sponsored by:
Computational Molecular Science and Engineering Forum

■ POLYMERS AND SOLVENTS

Paper 192a: Comparison of PRISM Theory and Molecular Dynamics Simulations for Studying Assembly in Block Copolymer Solutions of Varying Sequences and Composition — ***Ivan Lyubimov***, *Daniel J. Beltran-Villegas, Arthi Jayaraman*

Paper 192b: Molecular Dynamics of Inorganic and Polymer Interface with Force-Field Parameter Based on DFT Simulation — ***Hiroya Nitta***, *Kosuke Ohata, Kenta Chaki, Taku Ozawa*

Paper 192c: Comprehensive Generation of Libraries of Lignin Structures as an Exploration of Lignin Space — ***Lauren Dellon***, *Abraham Yanez-McKay, Wenjun Li, Ross Mabon, Linda J. Broadbelt*

Paper 192d: Understanding the Nanoscopic Structure of Lyotropic Liquid-Crystal Membranes Using Molecular Dynamics Simulations — ***Benjamin J. Coscia***, *Michael Shirts*

Paper 192e: Thermodynamics of Block Polymers: Monte Carlo Simulations and Self-Consistent Field Theory Study — ***Akash Arora***, *Frank S. Bates, Kevin D. Dorfman*

Paper 192f: Refinement of Techniques in Molecular Modeling of Multicompartment Nanoreactors — ***Kayla Hendrickson***, ***Nicholas Bond***, *SeungMin Lee, Connor Callaway, Parveen Sood, Seung Soon Jang*

Paper 192g: Rapid and Accurate Property Prediction for Polymer Systems Using Atomistic-Scale Simulation — ***Andrea R. Browning***, *Thomas J. L. Mustard, Jeffrey Sanders, Mathew D. Halls, Alexander Goldberg, H. Shaun Kwak, Stephen Christensen, Jacob Gavartin, Morisato Tsuguo*

Paper 192h: Flow Properties of Model Alkanes in Nanopores — ***Irais Valencia-Jaime***, *Caroline Desgranges, Jerome Delhommelle*

Paper 192i: Pure- and Mixed-Gas Absorption in Nonideal Binary Ionic Liquid Mixtures: A Molecular Simulation Study — ***Utkarsh Kapoor***, *Jindal K. Shah*

Paper 192j: Construction of a Hydrogel System for Bioadsorption and Bioseparations by Molecular Modeling and Simulation — ***Matthew Senter***, *Jee-Ching Wang*

Paper 192k: Modeling Alkane Partitioning and Phase Behavior in Non-Permeable and Permeable Slit Pores — ***Jinlu Liu***, *Walter G. Chapman*

Paper 192m: Molecular Dynamics of Waxy Crude Oil Under Magnetic Field — ***Xuejiao Chen***

Paper 192o: Enhancing the Oxidation of Toluene with External Electric Fields: A Reactive Molecular Dynamics Study — ***Shen Tan***, *Tao Xia, Yao Shi, Yi He*

Paper 192p: Molecular Simulation of Ionic Polyimides and Ionic Liquid Composites for Gas Separation — ***Asghar Abedini***, *C. Heath Turner, Jason E. Bara, Ellis Crabtree*

Paper 192q: Molecular Simulation of Ionic Liquid Mixtures: Applications to Capacitive Energy Storage — ***Matt Thompson***, *Katherine L. Van Aken, Robert Sacci, Justin Neal, Jianzhong Wu, Yury Gogotsi, Peter T. Cummings*

Paper 192r: Molecular Simulation of Ionic Liquid Systems: Effects of Solvation and Humidification — ***Matt Thompson***, *Felix Tiet, Naresh C. Otsi, Boris Dyatkin, Katherine L. Van Aken, De-en Jiang, Yury Gogotsi, Eugene Mamontov, Peter T. Cummings*

Paper 192s: Aerosol Formation in Post Combustion CO_2 Capture Columns: Molecular Dynamic Simulation — ***Dhawal Shah***, *Nardana Bazybek, Tomiris Boltaikhanova*

■ DRUG DISCOVERY AND BIOMOLECULES

Paper 192t: Molecular Simulation of Transport of DNA-Grafted Nanoparticles — ***James McLaughlin***, *Simona Ciobotarescu, Caroline Desgranges, Jerome Delhommelle*

Paper 192u: Protein Adsorption on Surfaces: The Role of Forcefield and Surface Ions — ***Arushi Prakash***, *Kayla Sprenger, Jim Pfaendtner*

Paper 192v: Scaling of Peptide Sequence-Dependent Hydrophobic Interactions from Experiment and Simulation — ***Jacob I. Monroe***, *Philipp Stock, Thomas Utzig, David J. Smith, Markus Valtiner, M. Scott Shell*

Paper 192w: Mapping of Gas Diffusion Pathways in [FeFe]-Hydrogenase — ***Mohammadjavad Mohammadi***, *Harish Vashisth*

Paper 192x: Studying the Structure and Dynamics of Amyloidβ(21–30) with Experiments and Simulations — ***Dilnoza Amirkulova***, *Maghesree Chakraborty, Andrew White*

Paper 192y: Solute Transport Across Blood-Brain Barrier Tight Junction Pores — ***Flaviyan Jerome Irudayanathan***, *Shikha Nangia*

Paper 192z: Capturing Differences in Dynamics of Structurally Similar Signaling Proteins — ***Hossein Mohammadiarani***, *Harish Vashisth*

Paper 192aa: Novel Computational/Experimental Approaches to DNA/Proteins Interactions — ***Sabrina Pricl***, *Erik Laurini, Maurizio Fermeglia, Domenico Marson, Enzo Di Fabrizio, Monica Marini*

Paper 192ab: Wiggling, Crowding, Self-Assembling: Synthesis and Activity of Computer-Designed Nanovectors for Gene and Drug Delivery — ***Erik Laurini***, *Maurizio Fermeglia, Silvia Brich, Domenico Marson*

Paper 192ac: New Anti-Mycobacterium Agents in Combination with P-gp Inhibitors: A Multidisciplinary Approach to Face an Old Re-Emerging Disease with New Tools — ***Erik Laurini***, *Suzana Aulic, Maurizio Fermeglia, Domenico Marson, Irene Briguglio, Roberta Ibba, Antonio Carta, Sabrina Pricl*

Paper 192ad: QSARs for Predicting Adipose: Blood Partitioning of Industrial Chemicals — ***Krystalia Papadaki***, *Spyros Karakitsios, Dimosthenis Sarigiannis*

Paper 192ae: Pharmacometabonomics Approach for Early Prediction of Neuropathy — ***Parul Verma***, *Jamie Renbarger, Jodi Skiles, Bruce Cooper, Doraiswami Ramkrishna*

■ MATERIALS, METALS, AND CATALYSTS

Paper 192af: A Theoretical Study of the Activation of Hydrogen and Methane by Frustrated Lewis Pairs — ***Marcos Becerra***, *Misael Real-Enriquez, Luis Rincon*

Paper 192ag: Differences in Relative Free Energy Versus Temperature Curves for Small Organic Molecules Between Quantum Mechanical and Classical Potentials — ***Natalie Schieber***, *Nathan Abraham, Eric Dybeck, Michael R. Shirts*

Paper 192ah: Density Functional Theory Screening of Metal Catecholates for Adsorption of Toxic Pnictogen Hydride Gases — ***N. Scott Bobbitt***, *Randall Q. Snurr*

Paper 192ai: Mechanism of Sodium Adsorption on N-Doped Graphene Nanoribbons — *Hong Woo Lee, Hye Sook Moon, Je Moon Yun, Kwang Ho Kim,* ***Seung Geol Lee***

Paper 192aj: Influence of Solvent on the Thermodynamics of Molecular Adsorption on Metal Surfaces — ***Tonnam Balankura***, *Kristen Fichthorn*

Paper 192ak: Molecular Simulation of Mechanical Properties of Multilayer Graphene Oxide Nanosheets — ***Xu Zhang***, ***Xiaoning Yang***

Paper 192al: Computational Discovery of New Materials and Processes for Industrial Separations — ***Mansi S. Shah***, *Michael Tsapatsis, J. Ilja Siepmann*

Paper 192am: Space-Charge Distribution Dynamics in Water-Splitting Photocatalytic $BiVO_4$ by Kinetic Monte Carlo Modeling — ***Viswanath Pasumarthi***, *Michel Dupuis*

Paper 192an: Molecular Simulations of Fullerene Stabilization in Water by Fullerene Oxides — ***Kendra Noneman***, *Eric Jankowski*

Paper 192ao: Interplay Between Crystallization and Glass Transition in Bimetallic Nanoalloys — ***Solene Bechelli***, *Caroline Desgranges, Jerome Delhommelle*

Paper 192ap: Molecular Simulations of Bubble Formation in Metastable Liquids — ***Brittany Gonzalez***, *Caroline Desgranges, Jerome Delhommelle*

Paper 192aq: Molecular Simulation of Gas Adsorption in Metal-Organic Frameworks — ***Gopalsamy Karuppasamy***, *Caroline Desgranges, Jerome Delhommelle*

Paper 192ar: Leveraging Heterostructural Alloying to Design Metastable Nitrides with Improved Piezoelectric Properties — ***Samantha L. Millican***, *Kevin Talley, Alan W. Weimer, Andriy Zakutayev, Charles B. Musgrave, Geoff Brennecka, Aaron Holder*

Paper 192as: Discovery of High-Performing MOFs via High-Throughput Computation and Machine Learning — ***Alauddin Ahmed***

Paper 192at: First-Principles Studies of the Interactions Between Chemical Species Inside Vanadium Redox Flow Batteries — ***Nadia N. Intan***, *Konstantin Klyukin, Vitaly Alexandrov*

Paper 192au: Dehydrogenation Mechanism of Liquid Organic Hydrogen Carrier Materials: A Density Functional Theory Study — ***Jae Yul Lim***, *Hyunguk Kwon, H. Shaun Kwak, Jeong Woo Han*

Paper 192av: The Crystal Structure and Surface Composition of Coalescing Ag-Au Nano-Alloys by Molecular Dynamics Simulations — ***Eirini Goudeli***, *Sotiris E. Pratsinis*

Paper 192aw: Hydrogen-Hydrate Cage-Hopping: Insights from Molecular Dynamics — *Christian Burnham, Zdenek Futera,* ***Niall J. English***

Paper 192ax: First-Principles Study of Atomistic Mechanisms in All-Vanadium Redox Flow Batteries — ***Zhen Jiang***, *Konstantin Klyukin, Vitaly Alexandrov*

Paper 192ay: Solvation Dynamics and Energetics of Single-Walled Carbon Nanotubes (SWCNTs) in Water/Alcohol Mixtures — ***Kevin R. Hinkle***, *Frederick R. Phelan Jr.*

Paper 192az: Effect of Liquid-Liquid and Solid-Liquid Interfacial Resistance on Heat Transfer in Nanomaterials — ***Sohail Murad***, *Ishwar K. Puri*

Paper 192ba: A Theoretical Investigation on NH_3, NO Diffusion and Sorption in ZSM5 Catalysts (MD and Monte Carlo simulation) — ***Sheida Jamalzadeh***, *Aligholi Niaei, Hamid Erfan nia, Amir Naser Shamkhali*

■ METHODS AND PARAMETER DEVELOPMENT

Paper 192bb: Multi-Metric 3D Protein Descriptors: The Correlation Impact of Algebraic Forms and Its Analysis — ***Julio Teran***, *Yovani Marrero-Ponce*

Paper 192bc: Accurate Methods to Describe System-Specific Polarization and Dispersion Energies — ***Thomas A. Manz***, *Nidia Gabaldon Limas, Taoyi Chen, Daniel J. Cole*

Paper 192bd: Applications of Atomistic Machine Learning for Estimating Adsorbate Free Energy and Entropy on Late-Transition Metal Surfaces — ***Prateek Mehta***, *Andrew Lehmer, Anshumaan Bajpai, Kurt Frey, William F. Schneider*

Paper 192be: Reconstructing Ancient Sequences to Understand the Structure and Function Relationships of Modern Proteins — ***Zahra Shamsi***, *Alexander Moffett, Diwakar Shukla*

Paper 192bf: Improved Thermal Gradient Quasiharmonic Approximations for Thermodynamic Properties of Organic Crystals with the Inclusion of Anisotropy — ***Nathan Abraham***, *Eric Dybeck, Natalie Schieber, Michael Shirts*

Paper 192bg: MOSDEF, a Python-Based Molecular Simulation and Design Framework — ***Justin Gilmer***, *Christoph Klein, János Sallai, Andrew Z. Summers, Christopher R. Iacovella, Ákos Lédeczi, Clare McCabe, Peter T. Cummings*

Paper 192bh: Screening Self-Assembled Monolayers for Lubrication Properties: Trends and Pitfalls — ***Christopher R. Iacovella***, *Christoph Klein, Trevor J. Jones, Clare McCabe, Peter T. Cummings*

Paper 192bi: Addressing Discrepancies in Hydrogen Abstraction by OOH Radical via Automatic Transition State Theory Calculations — ***Nathan Harms***, *Richard H. West*

Paper 192bj: Development of the Parallel Monte Carlo Simulation Engine GOMC — ***Mohammad Barhaghi***, *Jason R. Mick, Younes Nejahi, Yuanzhe Li, Loren Schwiebert, Jeffrey J. Potoff*

Paper 192bk: Machine Learning Approaches to Quantum Monte Carlo Challenges — ***Deidre Cleland***

Paper 192bl: Theoretical Study Energetic Ionic Salts Composed of Nitrogen Bridge 3,3'-dinitro-5,5'-bis-1,2,4-triazole-1,1'-diolate Anion and Various Cations — ***Guolin Xiong***, ***Weihua Zhu***, *Heming Xiao*

Paper 192bm: Structural Transformations and Absorption Properties of Crystalline4,10-dinitro-2,6,8,12-tetraoxa-4,10-diazaisowurtzitane under High Pressures — ***Dong Xiang***, ***Weihua Zhu***

(193) Poster Session: Engineering Fundamentals in Life Science
Monday, Oct 30, 3:15 PM
MCC, Exhibit Hall B

Kris N. Dahl, Chair
Roger G. Harrison, Co-Chair
David M. Umulis, Co-Chair

Sponsored by:
Engineering Fundamentals in Life Science

Paper 193a: N-Terminal Hypothesis for Alzheimer's Disease: Arguments for and Against — *Brian Murray, Bhanushee Sharma, Srivathsan V. Ranganathan,* ***Georges Belfort***

Paper 193b: Modeling Alzheimer's Disease Using Cortical Organoids Derived from Human Induced Pluripotent Stem Cells — ***Yuanwei Yan***, *Julie Bejoy, Liqing Song, Yi Zhou, Yan Li*

Paper 193c: pH-Dependent PDGF-BB-Induced Chemokinesis and Chemotaxis of NIH 3T3 Fibroblasts and Rat Bone Marrow–Derived Mesenchymal Stem Cells — ***Nhat-Anh N. Tong***, *Long Quang Pham, David Chege, Timothy Dijamco, Sagnik Basuray, Roman Voronov*

Paper 193d: Investigation of the Variation in Exosome Release by Human Pluripotent Stem Cells in Static and Stirred Suspension Cultures — *Preeti Ashok,* ***Emmanuel S. Tzanakakis***

Paper 193e: Differential Expression of Neuron-Glial Antigen 2 (NG2) and Melanoma Cell Adhesion Molecule (CD146) in Mesenchymal Stem Cells — ***Kim O'Connor***, *Katie Russell, Alan Tucker, Bruce Bunnell, Michelle Lacey, Michael Andreeff*

Paper 193f: Heterotypic Cell-Cell Interactions of Human Induced Pluripotent Stem Cells and Human Mesenchymal Stem Cells for Neural Differentiation — ***Liqing Song***, *Ang-Chen Tsai, Xuegang Yuan, Julie Bejoy, Sebastien Sart, Teng Ma, Yan Li*

Paper 193g: Development of HER2-Positive Breast Tumor Spheroids as a Better Approach to Study the Effectiveness of Novel Anticancer Therapies — *Celia Nieto, Gema Marcelo, Miguel A. Galán,* ***Eva Martín del Valle***

Paper 193h: Construction of a Multi-Culture Human Lung Platform for Tumor Metastasis Study — *Bing-Syuan Ni,* ***Jen-Huang Huang***

Paper 193i: Enhanced Cancer Immunotherapy by Chimeric Antigen Receptor-Modified T Cells Engineered to Secrete Checkpoint Inhibitors — ***Natnaree Siriwon***, *Si Li, Yu-Jeong Kim, Pin Wang*

Paper 193j: Combination Cancer Therapy Using Chimeric Antigen Receptor Engineered Natural Killer Cells as Drug Carriers — ***Elizabeth Siegler***, *Yu Jeong Kim, Xianhui Chen, Pin Wang*

Paper 193k: Investigating the Drug Delivery Effect for Anti-Cancer Compounds Using Graphene Oxide Nanoparticles — ***Linh Doan***, *Tracy J. Benson*

Paper 193l: The Regulation of Macrophage Phagocytic Engulfment by Glioblastoma Cell Secreted Factors — ***Nisha G. Sosale***, *Matthew J. Lazzara*

Paper 193m: Genetic Polymorphisms in Inflammasome-Dependent Innate Immunity Among Pediatric Patients with Severe Renal Parenchymal Infections — ***Chi-Hui Cheng***, *Yun-Shien Lee, Jui-Che Lin*

Paper 193n: Therapeutic Effect of Inhaled Tacrolimus-Loaded Nanocomposite Microparticles (nCmP) in a Pulmonary Hypertension–Induced Rat Model — ***Sweta K. Gupta***, *Alexander Vang, Nishan Shah, Nouaying R. Kue, Zimeng Wang, Gaurav Choudhary, Samantha A. Meenach*

Paper 193o: Metabolomics as a Quality Control Tool for Chondrogenic Differentiation in Spheroids: From Microaggregates to Microtissues — ***Niki Loverdou***, *Gabriella Nilsson-Hall, Ioannis Papantoniou, Liesbet Geris*

Paper 193p: Engineering the Endothelial Glycocalyx to Restore Its Structure and Function — ***Eno E. Ebong***, *Solomon Mensah, Ming Cheng*

Paper 193q: Single-Cell Profiling of Dynamic Cytokine Secretion and the Phenotype of Immune Cells — ***Xingyue An***, *Victor G. Sendra, Ivan Liadi, Balakrishnan Ramesh, Gabrielle Romain, Melisa Martinez-Paniagua, Maksim Mamonkin, Navin Varadarajan*

Paper 193r: Influence of Hepatic Function Due to Co-Culturing with Endothelial Cell from Different Tissue Origins — ***Carrie German***, *Sundararajan V. Madihally*

Paper 193s: An All-in-One High-Throughput Microfluidic Platform for Cell Culture and Migration Control — ***Long Quang Pham***, *Paul Abatemarco, Timothy Dijamco, David Chege, Roman Voronov*

Paper 193t: Sustained Delivery of Phosphates from Crosslinked PEG Hydrogel Nanoparticles Suppress Collagenase Activity of Intestinal Pathogens — ***Dylan Nichols***, *Olga Zaborina, John Alverdy, Seok Hoon Hong, Fouad Teymour, Georgia Papavasiliou*

Paper 193u: Towards Structure-Based HIV Vaccine Design: Exploring the V1V2 Loop Conformational Landscape with Protein Engineering — ***Chris Bailey-Kellogg***

Paper 193v: Coarse-Grained Molecular Simulations Reveal Regulatory Insights into Immature HIV-1 Assembly Dynamics — ***Alexander J. Pak***, *John M. A. Grime, Gregory A. Voth*

Paper 193x: Multidrug-Resistant *Escherichia coli*: Measurement of Membrane Mechanical Properties, Nanoscale Adhesion, and Biofilm Formation — ***Samuel Uzoechi***, *Nehal Abu-Lail*

Paper 193y: Bacterial Cellulose: Self-Assembly and Reformatting — ***Sierin Lim***

Paper 193z: Mechanical Force-Based Regulation of Protein Assemblies — ***Ravi Chawla***, *Katie Ford, Pushkar Lele*

Paper 193aa: Multiscale Analysis of Autotroph-Heterotroph Interactions in a High-Temperature Microbial Community — ***Kristopher Hunt***, *Ryan Jennings, William Inskeep, Ross P. Carlson*

Paper 193ab: A Parallel Framework for Systematic Development of Multiscale Models Bridging Subcellular Biochemistry to Cell Population Dynamics — ***Mohammad Islam***, *Satyaki Roy, Sajal Das, Dipak Barua*

Paper 193ac: Development of Mathematical Approach to Studying Cholesterol Deposition in the Artery for Different Fluid Models — ***Abbas Motamedilamouki***, *Pedro E. Arce, J. Robby Sanders*

Paper 193ad: Progenitor Cell Isolation Using MMP-Degradable Hydrogels for Heart Disease Therapy — ***Calvin F. Cahall***, *Brad Berron*

Paper 193ae: Noninvasive Diagnostics for the Early Detection of Lower Respiratory Diseases: An In-Silico Study — ***Yu Feng***, *Jun Wang, Xiaole Chen*

Paper 193af: Fabrication of In-Vitro Human Breathing Lung Model for Inhalation Drug Development — *Chun-Kai Lin, Pulak Nath,* ***Jen-Huang Huang***

Paper 193ag: Screening of Natural Osmolytes for Inhibiting Cancer-Causing p53 Hot Spot Mutant Peptides Aggregation — *Zhaolin Chen,* ***Mathumai Kanapathipillai***

Paper 193ah: Comprehensive Molecular Classification of Cell Types and Cell Type–Specific Response to Tissue Injury Using Massively Parallel Single-Cell Genomics — ***Karthik Shekhar***

Paper 193ai: Novel Role of Transmembrane Domain of IRE1α Protein During Activation and Its Implications in Progression of Cancer — ***Amrita Oak***, *Christina Chan*

Paper 193aj: Validation of a Population Balance Model for Tumor Growth Using Zebrafish Melanoma Experiments — ***Adeyinka Lesi***, *Silja Heilmann, Richard White, David Rumschitzki*

Paper 193ak: Modeling of Fluid Flow and Oxygen Distribution in Solid Tumors — ***Moath Alamer***, *Xiao Yun Xu*

Paper 193al: Optimization of Vincristine Infusion Time — ***Parul Verma***, *Yuqi Fang, Doraiswami Ramkrishna*

Paper 193am: Quantitative *in vivo* & *ex vivo* multimodality cell imaging of antigen-specific T-cells in murine metastatic ovarian cancer — ***Matthew Willadsen***, *Iven Yarovoy, An Qi Zhang, Steven Turowski, Joseph Spernyak, Mukung Seshadri, A.J. Robert McGray, Kunle Odunsi, Natesh Parashurama*

Paper 193an: Engineering the liver diverticulum from human pluripotent stem cells — ***Ogechi Ogoke***, *Cortney Ott, Natesh Parashurama*

Paper 193ao: Controlling Endodermal Cell State by Understanding and Re-engineering Developmental Master Regulatory Gene Circuits — ***Saber Meamardoost***, *Natesh Parashurama*

(194) Poster Session: Food and Bioprocess Engineering
Monday, Oct 30, 3:15 PM
MCC, Exhibit Hall B

Nuttha Thongchul, Chair
Xiaorui Yang, Co-Chair
Mengmeng Xu, Co-Chair

Sponsored by: Food

■ BIOENGINEERING

Paper 194a: Modeling Drug Delivery by Electrokinetic-Based Methods in Cancer Tumor Treatment — ***Samantha Blanton***, *A. Nastasia Allred, Pedro E. Arce, J. Robby Sanders*

Paper 194b: Ex-Vivo Study of Nanowires in Miniguts — *Yijun Qi, Enzheng Shi, Nathan Peroutka-Bigus, Bryan Bellaire, Michael J. Wannemuehler, Albert Jergens, Terrence Barrett, Yue Wu,* ***Qun Wang***

Paper 194c: Comprehensive Proteomic Analysis of High-Productivity CHO Cells — ***Ningning Xu***, *Chao Ma, Kahyong Goh, Jianfa Ou, Lufang Zhou, Xiaoguang Liu*

Paper 194d: Labeling Neural Stem Cells Using Trackable Ultrasmall Iron Oxide Nanoparticle for Cell Transplantation Therapy — ***Seungjo (Joe) Park***, *Jennifer Sherwood, Yuping Bao, Yonghyun (John) Kim*

Paper 194e: Using RNA-Seq to Investigate Population Heterogeneity Among Human Pluripotent Stem Cells Cultured on 2D or in 3D Biomaterial Scaffolds — ***Maroof M. Adil***, *David V. Schaffer*

Paper 194f: Screening and Characterization of Rabbit scFv Antibodies for Sensitive Detection of C-Reactive Protein in Clinical Diagnosis — *Jun-ichi Horiuchi,* ***Yoichi Kumada***

Paper 194g: Understanding the Effects of Ultrasound on *Pseudomonas aeruginosa* Bacterial Biofilms — *Lakshmi Deepika Bharatula,* ***James J. Kwan***

Paper 194h: Optical Nanosensors for Monitoring 3D Oxygen Gradients and Oscillations in Biofilms — *Megan Jewell, Anne Galyean,* ***Kevin J. Cash***

Paper 194i: Rapid and Facile Fabrication of Thermoplastic Organs-on-Chips — ***Sanjin Hosic***, *Shashi Murthy, Abigail Koppes*

Paper 194j: Byproduct Cross-Feeding and Community Stability in an In-Silico Biofilm Model of the Gut Microbiome — *Michael A. Henson,* ***Poonam Phalak***

■ FOOD

Paper 194k: Mathematical Modelling of Salt Transport in Dry Salted Cheeses — ***Meghan Keck***

Paper 194l: Optimization of Aqueous Extraction Conditions of Tannin from Quercus infectoria Galls — ***Harisun Yaakob***

Paper 194m: Effect of Drying Temperature, Humidity and Time on the Physico-Chemical Properties of Sugar Kelp (*Saccharina latissima*) — ***Praveen Sappati***, *Emily DuranFrontera, Balunkeswar Nayak, G. Peter van Walsum*

Paper 194n: Stability of Virucidal Effects of Green Tea Extracts — ***Jinku Kim***

Paper 194o: Exploring the Potential Applications of Molecular Simulations to the Food Industry — ***Panagiota Kyriakou***

Paper 194p: Assessing Environmental Impact from Acid Whey to Value-Added Products — *Jasmina Burek, Daesoo Kim, Peggy M. Tomasula, Winnie C. F. Yee,* ***Greg Thoma***

Paper 194q: Value-Added Products from Agro-Industrial Wastes: Colombian Andes Berry (*Rubus glaucus*) Residues — ***Javier Davila Sr.***, *Gonzalo Taborda Sr., Moshe Rosenberg, Carlos Ariel Cardona Alzate*

■ MEMBRANE

Paper 194r: Fe(III)-Induced Rapid Deposition and Polymerization of Dopamine on Microfiltration (MF) Membranes — ***Xuehua Ruan***, *Xuhang Liao Sr., Yan Dai, Xiaobin Jiang,* ***Gaohong He***

Paper 194s: Crystal Morphology–Modified and Solution Recovery–Improved Membrane Crystallization — ***Xiaobin Jiang***, *Dapeng Lu, Guannan Li,* ***Gaohong He***

■ BIOPROCESSING

Paper 194t: Engineer Bacteria Consortia to Execute Concerted Enzymatic Reactions — ***Qing Sun***, *Timothy Lu*

Paper 194u: Effect of Heat Stress on Rice Seed Development: Discovering Global Regulatory Players and Modeling of Rice Metabolism — ***Rajib Saha***, *Mohammad Mazharul Islam, Harkamal Walia, Jaspreet Sandhu*

Paper 194v: Characterization and Heterologous Expression of Iron Hydrogenase Ethha_0031 of *Ethanoligenens harbinense* in *E. coli* BLR(DE3) — ***Weiming Li***, *Chi Cheng, Shang-Tian Yang, Nanqi Ren*

Paper 194w: Metabolic Engineering of *Clostridium aceticum* for Acetone, Butanol and Ethanol Fermentation — ***Chi Cheng***, *Shang-Tian Yang*

Paper 194x: A Novel Technique for the Usage of Agricultural Solid Substrate Extract for the Production of Valuable Therapeutic Enzymes — ***Anup Ashok***, *Vaibhav Lendekar, Santhosh Kumar Devarai*

Paper 194y: The Enhanced Butanol Production and High-Efficient Product Recovery with Reduced Wastewater Generation — ***Chuang Xue***

Paper 194z: Suite of Bacteria from the *Enterobacter* Genus Suitable for Lignin Degradation — ***John Nicpon***, *Rajesh Shende, Anuradha Shende*

Paper 194aa: Decoding Icy Metabolism: Flux Topology of a Psychrophilic Extremophile — ***Jeffrey Czajka***, *Whitney D. Hollinshead, Yinjie Tang*

Paper 194ab: Metabolic Engineering of Tobacco for the Production of the Anti-Cancer Drug Etoposide — ***Bailey Schultz***, *Warren Lau, Elizabeth Sattely*

Paper 194ac: CRISPR-Mediated Genome Editing and Gene Repression in *Scheffersomyces stipitis* — ***Mingfeng Cao***, *Meirong Gao, Deon Ploessl, Zengyi Shao*

Paper 194ad: Application of the Genome-Scale Modeling Approach to Exoelectrogenic Microorganisms in Microbial Fuel Cells — ***Robert Hanes Jr.***, *Zuyi (Jacky) Huang*

TECHNICAL SESSIONS 2017

Paper 194ae: Multi-Paradigm Multiscale Metabolic Modeling of a Nitrogen-Fixing Cyanobacterium with Two Distinct Metabolic Modes — *Joseph Gardner, Bri-Mathias S. Hodge,* ***Nanette R. Boyle***

Paper 194af: Modeling of Stationary Phase in Microalgae Growth Using the Population Balance Equation — ***Ergys Pahija****, Chi Wai Hui*

Paper 194ag: Uncovering and Correcting the Effect of Biomass Molecular Weight Discrepancies in FBA Calculations — ***Siu Hung Joshua Chan****, Jingyi Cai, Lin Wang, Margaret Simons-Senftle, Costas D. Maranas*

Paper 194ah: Anaerobic Digestion of Kitchen Waste to Produce Biogas — ***Mai Khalfan Salem Al Daeiri****, Alaa Mohammed Al Sheikh Faiyadah, Zahra Khalfan Mabrook Al Amri, Marwa Al Alwai, Avnish Pareek, Hesham El-Enshasy*

Paper 194ai: Elucidation of Carbon Flux Topology Representing Photoautotrophic Growth in Synechocystis PCC 6803 Using Genome-Scale Isotopic Instationary Metabolic Flux Analysis — ***Saratram Gopalakrishnan****, Himadri B. Pakrasi, Costas D. Maranas*

Paper 194aj: N-acetylchitohexaose Producing Chitinase Identified from Chitinase Profiles of Aeromonas schubertii by Enzymomics, a Novel Technique — ***Chao-Lin Liu****, Jeen-Kuan Chen, Yu-Kuo Liu*

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(195) Poster Session: Interfacial Phenomena (Area 1C)
Monday, Oct 30, 3:15 PM
MCC, Exhibit Hall B

Raymond Tu, Chair
Raymond R. Dagastine, Co-Chair

Sponsored by: Interfacial Phenomena

Paper 195a: Characterization of Orientation and Photochemical Function of Chlorophyll a Molecules in Self-Assembled Membranes — ***Shogo Taguchi****, Keishi Suga, Keita Hayashi, Yukihiro Okamoto, Hidemi Nakamura, Hiroshi Umakoshi*

Paper 195b: Design of Lipid Membrane Surfaces as Organocatalyst for Michael Reactions in Aqueous Media — ***Masanori Hirose****, Keishi Suga, Yukihiro Okamoto, Hiroshi Umakoshi*

Paper 195c: A Unified Structure-Property Relationship for Alkyl-Polyoxide Surfactants — ***Zachary R. Hinton****, Nicolas J. Alvarez*

Paper 195d: Relating Rheology with Morphology: Cholesterol in a Model Lung Surfactant Monolayer — *Steven Patton, Amit Kumar Sachan, Ian Williams, Todd M. Squires,* ***Joesph A. Zasadzinski***

Paper 195e: A MATLAB-Based Tool Package for Interfacial Property Calculations — ***Xiaoqun Mu****, Walter G. Chapman, Florian Frank, Faruk O. Alpak*

Paper 195f: Thermodynamics Study of Silica Precipitation in a Hydrometallurgical Process — ***Christian Manfoumbi***

Paper 195g: Interfacial Phenomena During Biomass Pyrolysis — ***Saurabh Maduskar****, Christoph Krumm, Paul J. Dauenhauer*

Paper 195h: Food-Grade Surfactant Blends for Stabilization of Oil and Water Emulsions — ***Patricia Valenzuela****,* ***Anju Gupta***

Paper 195i: Interaction forces between colliding emulsion drops (Oil or Water) coated with non-ionic surfactants (C12E5 and PGPR) — ***Srinivas Mettu****, Joseph D. Berry, Chu Wu, Raymond R. Dagastine*

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(196) Poster Session: Materials Engineering & Sciences (08A — Polymers)
Monday, Oct 30, 3:15 PM
MCC, Exhibit Hall B

Megan L. Robertson, Chair
Julie Albert, Co-Chair
Jeffrey Rimer, Co-Chair

Sponsored by: Materials Engineering and Sciences Division

Paper 196a: Theoretical Study of the Reaction Kinetics of Organosiloxane Polycondensation — ***Mona Bavarian****, Siamak Nejati*

Paper 196c: Control Strategy and Comparison of Tuning Methods for Continuous Lactide Ring-Opening Polymerization — ***L. Ivano Costa****, Ulla Trommsdorff*

Paper 196d: From Process to Product: Enhancing the Understanding of α-Olefin-Polymerizations — *Kristina M. Pflug, Jonas Nowottny,* ***Markus Busch***

Paper 196e: Amine Effects on Radial-Mediated Thiol-Ene Reactions — ***Dillon Love****, Kang-Min Kim, Johnathan Goodrich, Benjamin D. Fairbanks, Mark Stoykovich, Charles B. Musgrave, Christopher Bowman*

Paper 196f: Influence of Phosphate Salts and Solution pH on Aqueous-Phase NVP Free-Radical Polymerization — ***Fernando T. P. Borges****, Fouad Teymour*

Paper 196g: Synthesis of Sustainable Polyesters from Bio-Derived Fatty Acids — ***Aditya Banerji****, Mahesh Mahanthappa, Christopher J. Ellison*

Paper 196h: Synthesis and Characterization of Crosslinked Polymers from Cottonseed Oil — *Rangana Wijayapala, Deonante Frazier, Bill B. Elmore, Charles Freeman,* ***Santanu Kundu***

Paper 196i: Date Pits as Cost-Effective, Renewable, and Efficient Fillers for Polymers — ***Fares Alsewailem****, Yazeed Binkhodor*

Paper 196j: Biaxial and Shear Deformation of Simulated Amorphous Cis-, Trans-1, 4-Polybutadiene Chains — ***Suvrajyoti Kar****, Michael L. Greenfield*

Paper 196k: Decomposition Behavior of Laponite/PLGA-PEG-PLGA Nanocomposite Hydrogels at Body Temperature — ***Midori Kitagawa****, Tomoki Maeda, Atsushi Hotta*

Paper 196l: Synthesis of Thermoplastic Polydimethylsiloxane with L-Phenylalanine-Based Hydrogen-Bond Network and Its Self-Healing Property — ***Shunsuke Tazawa****, Atsushi Shimojima, Tomoki Maeda, Atsushi Hotta*

Paper 196n: Controlled Swelling Rate Elastomer for Packers — ***Rostyslav Dolog****, Darryl Ventura, Valery N. Khabashesku, Qusai Darugar*

Paper 196o: Effect of the Cross-Linking Agent (Sodium Polyphosphate) on Performances of NaCS-WSC Microcapsules — ***Qing-Xi Wu****, Yi-Xin Guan, Jun-Jie Yuan, Shan-Jing Yao*

Paper 196p: Swelling Behaviors of Cr(III)-Modified Acrylamide-Based Superabsorbent Polymer Microsphere in Brines — ***Jingyang Pu****, Jiaming Geng, Na Zhang, Baojun Bai*

Paper 196q: Synthesis of Chemical Protective Elastomeric Barrier Materials — ***James Ogilvie-Battersby****,* ***Alessandra Molinaro****, Christopher Zoto, Quoc Truong, Nese Orbey*

Paper 196r: Polysulfide-Based Nanofiber Prepared via Inverse Vulcanization and Electrospinning for Effective Mercury (II) Sequestration — ***Lawrence A. Limjuco****, Grace M. Nisola, Khino J. Parohinog, Kris Niño G. Valdehuesa, Wook-Jin Chung*

Paper 196s: Synthesis and Characterization of Charged Polymer/Graphene Oxide Composite Membranes for Water Purification — ***Szu-Ming Yang****, Heonjoo Ha, Christopher J. Ellison*

Paper 196t: Development and Analysis of a Thin-Film Nanocomposite Membrane: Resistance to Chlorine — ***Abdulmajeed Altalhi****, Holly Stretz*

Paper 196v: Antimicrobial Polymers: Present State of the Art — ***Nikhil Prakash***

Paper 196w: Layer-by-Layer Coated Microneedle Arrays for Staged Multi-Agent Immune Attack on Melanoma — ***Yanpu He****, Jiahe Li, Hongkun He, Celestine Hong, MayLin Funkenbusch, Sheryl Wang, Maya Berlinger, Darrell J. Irvine, Paula T. Hammond*

Paper 196x: Direct Observation of Remarkable Nanoparticle Evolution During Aqueous Dissolution of Polymer/Drug Particles — ***Ralm Ricarte****, Marc A. Hillmyer, Timothy P. Lodge*

Paper 196y: Polymerized Ionic Liquid Pentablock Terpolymer for Lithium-Metal Batteries — ***Tzu-Ling Chen****, Yossef A. Elabd*

Paper 196z: Effect of Electric Field on the Structure and Dynamics of Model Ionomer Melts — ***Janani Sampath****, Lisa M. Hall*

Paper 196aa: High-χ Block Copolymers with High Etch Selectivity for Sub-10 Nm Patterning — ***Sung-Soo Kim****, Walter W. Young, Luis E. Oquendo, Michael Maher, Sunshine X. Zhou, Yusuke Asano, Marc A. Hillmyer, C. Grant Willson, Christopher J. Ellison*

Paper 196ab: Fabrication and Structural Analysis of Nanofibers Made by Syndiotactic Polypropylene with Ethylene-Comonomer Units — ***Fuyuaki Endo****, Claudio De Rosa, Atsushi Hotta*

Paper 196ac: Role of Compatibilizer in 3D-Printed Objects — ***Matthew Spreeman****, Holly A. Stretz*

Paper 196ad: Interaction Between Supercritical CO_2+Cosolvent and Poly(vinyl acetate) — ***Dong-dong Hu****, Lei Bao, Ling Zhao, Tao Liu*

Paper 196ae: Modeling of Distributions of Polymer Properties Using Parallel Computing in Julia — ***Esteban Pintos****, Mariano Asteasuain*

Paper 196af: Transition Metal–Based Nanocrystals Confined Growth on Heteroatom-Doped Graphene Toward Hydrogen Catalysis — ***Minghao Zhuang****, Zhengtang Luo*

(197) Poster Session: Materials Engineering & Sciences (08B — Biomaterials)
Monday, Oct 30, 3:15 PM
MCC, Exhibit Hall B

Megan L. Robertson, Chair
Jeffrey Rimer, Co-Chair

Sponsored by: Materials Engineering and Sciences Division

Paper 197a: Influence of Molecular Design on the Self-Assembly of Single-Stranded DNA Amphiphiles — ***Thomas Gartner III****, Huihui Kuang, Efrosini Kokkoli, Arthi Jayaraman*

Paper 197b: Intracellular Trafficking of Enzyme-Cleavable Peptide Amphiphiles — ***Handan Acar****, James L. LaBelle, Matthew V. Tirrell*

Paper 197c: Polylactide-Based Biodegradable Zwitterionic Polymers and Their Conjugates with Drugs for Biomedical Applications — ***Haotian Sun****, Michael Yu Zarng Chang, Wei-I Cheng, Qing Wang, Alex Commisso, Meghan Capeling, Yun Wu, Chong Cheng*

Paper 197d: Overcoming Obstacles to Brain Repair Using Biomaterials — ***Tatiana Segura***

Paper 197e: A High-Throughput, Quantitative 3D Multi-Particle Tracking Model Demonstrates Regional Dependence of Nanoparticle Diffusion in the Brain — ***Chad D. Curtis****, Mike McKenna, Elizabeth Nance*

Paper 197f: Layer-by-Layer Nanoparticles for Interleukin-12 Delivery — ***Antonio E. Barberio****, Santiago Correa, Erik Dreaden, Talar Tokatlian, Mariane B. Melo, Darrell J. Irvine, Paula T. Hammond*

Paper 197g: Implantable Biomaterials Produced by Complexing Chitosan to Alginate or Pectin: Surface Properties, Hemocompatibility and Cytotoxicity — ***Fernanda C. Bombaldi de Souza****,* ***Renata F. Bombaldi de Souza****, Ângela Maria Moraes, Diego Mantovani*

Paper 197h: Development of Sustainable Therapeutic Dressings Consisting of Chitosan-Alginate Films Incorporating *Arrabidaea chica* Verlot Extract — *Ana Luíza Resende Pires, Cecília Buzatto Westin, Ilza Maria de Oliveira Sousa, Mary Ann Foglio,* ***Ângela Maria Moraes***

Paper 197i: Comparison of Chitosan Particles Produced by Ionic Gelation and by Supercritical Assisted Atomization — *Júlia Natalia Oliveira Mazoni,* ***Paulo de Tarso Vieira e Rosa***

Paper 197j: Exploiting a Novel Aqueous-Two Phase Microfluidic System for Cell Encapsulation in GAG+Chitosan Microcapsules — ***Amin Vossoughi Shahvari****, Howard W. T. Matthew*

Paper 197k: Laser-Activated Nanocomposites for Tissue Repair — ***Russell Urie****, Deepanjan Ghosh, Mitzi Thelakkaden, Tanner Flake, Jerry Crum, Chengchen Guo, Jeff Yarger, Kaushal Rege*

Paper 197l: New Strategy for the Fabrication of Annular Cylindrical Polysaccharide-Based Scaffolds — ***Ângela Maria Moraes****, Renata F. Bombaldi de Souza, Fernanda C. Bombaldi de Souza*

Paper 197m: Formulation of Peptide Antimicrobials for Treatment of Wound Infections — *Ritu Goyal, Michael Holloway, Pooja Patel, David Devore,* ***Charles Roth***

Paper 197o: Synthesis and Degradation of Biodegradable Copolymers — ***Eswar Arunkumar Kalaga****, Timothy Brenza*

Paper 197p: Light-Driven Ion Transport Using Biomimetic Membranes — ***Cory Jones****, Hasin Feroz, Manish Kumar*

Paper 197q: Exploring the Mechanisms of Bone Remineralization — ***Sanjana Epari***

Paper 197r: Ultra-High-Surface-Area Activated Carbon from a Renewable Resource — ***Ashli Polanco****, Dmytro Volkov, Quoc Truong, Carl Lawton, Nese Orbey*

Paper 197s: Improve Bio-Wettability of Ti-6Al-4V Alloys — ***Ashwin Kumar***

Paper 197t: A Facile Novel Fluorocarbon Copolymer Solution Coating Process for Improving Platelet Compatibility of Titanium — *Sophia Chao-Wei Huang, Chi-Hui Cheng, Yun Chiu, Yi-Ching Lin,* ***Jui-Che Lin***

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(198) Poster Session: Materials Engineering & Sciences (08D — Inorganic Materials)
Monday, Oct 30, 3:15 PM
MCC, Exhibit Hall B

Megan L. Robertson, Chair
Jeffrey Rimer, Co-Chair

Sponsored by: Materials Engineering and Sciences Division

Paper 198a: Alignment of Quantum Dot Nanorod/Silica Hybrid Particles on Glass Substrate for Luminescent Solar Concentrator — ***Kiju Um****, Young-Geon Song, Kangtaek Lee*

Paper 198b: Effect of Graphene Oxide on Formation of Zirconium Tungstate Nanoparticles — ***Young-Geon Song****, Kiju Um, Kangtaek Lee*

Paper 198c: Hierarchical $NiCo_2O_4$ Nanosheets on Carbon Nanofiber Films for High–Energy Density and Long-Life Li-O_2 Batteries — *Guoxue Liu,* ***Lei Zhang****, Suqing Wang, Liang-Xin Ding, Haihui Wang*

Paper 198d: Rapid Microwave-Assisted Synthesis of Hybrid Zeolitic-Imidazolate Frameworks — ***Febrian Hillman****, John Zimmerman, Seung-Min Paek, Mohamad Hamid, Woo Lim, Hae-kwon Jeong*

Paper 198e: Facile Synthesis of Cd-Substituted Zeolitic-Imidazolate Framework Cd-ZIF-8 and Mixed-Metal CdZn-ZIF-8 — ***Jingze Sun****, Hae-Kwon Jeong, Woo Taik Lim, Liya Semenchenko*

Paper 198f: A Study of Asymmetry Cu-MOFs Electrode Prepared In Situ and Its Biomimetic Catalysis — ***Zhipeng Li****, Liwei Ren, Diannan Lu*

Paper 198g: Protected SiC Catalyst Support for Steam Methane Reforming Reaction — ***Naftali Opembe****, Seungdoo Park, Sergio Ibanez, Doug Mitchell, Matthew Seabaugh, Scott Swartz*

Paper 198h: Computational Screening of High-Temperature Materials for Environmental Barrier Thin Films — ***Amanda Hoskins****, Aidan Coffey, Charles B. Musgrave, Alan W. Weimer*

Paper 198i: Phase Transformation Induced by Tetragonality Variation of Metal-Redox Synthesised NiMn Nanoalloys — ***Jian Shen****, Xin Jin*

Paper 198j: Fabrication of Electrospun Mesoporous Silica Nanomaterials for Water Vapor Adsorption — ***Soyoung Kim****, Heechul Choi*

Paper 198k: Applications of Mesoporous $RuCo_2O_4$ Thin Film for High-Performance Supercapacitor — ***Do-Heyoung Kim****, Nilesh R. Chodankar*

Paper 198l: TiO_2 Thin-Film Deposition by Electrospray — ***Yaqun Zhu,*** *Jong Hyun Shim, Junghyun Cho, Paul R. Chiarot*

Paper 198m: Green Synthesis of Copper Oxide Nanoparticles Using a Simple Microwave-Assisted Method — ***Prasad P. Pawar****, Shishir V. Kumar, Adarsh Bafana, Ashiqur Rahman, Si A. Dahoumane, Clayton S. Jeffryes*

Paper 198n: Comprehensive Thermodynamic Modeling of Mixed-Solvent Electrolyte Systems: An Investigation on the Quaternary System of $FeCl_2$-$FeCl_3$-HCl-H_2O — ***Sina Hassanjani Saravi****, Chau-Chyun Chen*

Paper 198o: Controllable Manipulation of Continuous AFI Membranes with Distinctive Microstructures on Macroporous Alpha-Alumina Substrates — *Hongfeng Dong, Xiufeng Liu,* ***Huiming Zhu****, Baoquan Zhang*, Jian Li*

Paper 198p: Magnetic Core-Shell Microspheres for Extraction of Rare Earth Elements from Geothermal Brine Solution — ***B. Peter McGrail****, Jian Liu*

Paper 198q: Three-Dimensional Finite Element Analysis of Self-Propagating High-Temperature Synthesis of Solid Oxide Fuel Cell Cathode Material — ***Venkata V. K. Doddapaneni****, Sidney Lin*

Paper 198r: Encapsulation of Dye in NH_2-UiO-66 Metal-Organic Framework for Photosensitized Oxidation of Benzyl Alcohol — ***Xiyi Li,*** *Qingqing Hou, Neng Liao,* ***Jing Xiao***

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(199) Poster Session: Materials Engineering & Sciences (08E — Electronic and Photonic Materials)
Monday, Oct 30, 3:15 PM
MCC, Exhibit Hall B

Megan L. Robertson, Chair
James Dorman, Co-Chair
Jeffrey Rimer, Co-Chair

Sponsored by: Materials Engineering and Sciences Division

Paper 199a: The Fabrication of Graphene/Polyaniline Blended Fiber for Conducting and Flexible Energy Storage Devices — *Yafei Feng, Jiaxin Shen, Cunliang Ma,* ***Yidong Liu****,* ***Yong Min***

Paper 199b: Semiconducting Heterostructures for Photocatalytic Reduction of Carbon Dioxide — ***Debtanu Maiti****, Johnnie Cairns, J. N. Kuhn, Venkat R. Bhethanabotla*

Paper 199c: Photoswitchable Quantum Dots Probes for Superresolution Microscopy — ***Abhilasha Dehankar****, Kil Ho Lee, Abhijeet Marar, Karine Thate, Carol Lynn Alpert, Peter Kner, Jessica O. Winter*

Paper 199d: Bottom-Up Synthesis of Nanoelectronic Titania Composites — ***Yang Lu****, Evan K. Wujcik, Arijit Bose*

Paper 199e: Synthesis and Characterization of ALD-Deposited Thin Films of Aluminum Oxides, Nickle Oxides, and Cobalt Oxides for Rectenna-Based Heat Harvesters — ***Xianglei Li****, Zachary Thacker, Patrick J. Pinhero*

Paper 199f: Combinatory Approach to Find Multi-Component Thermoelectric Material with High Power Factor — ***Wei Zheng***

Paper 199g: Manipulating Electrical and Thermal Transport in Bulk Nanostructured Materials — ***Yue Wu***

Paper 199h: Phase Diagrams, Defect Models and Thermoelectric Properties: ß-Ag_2se and $CoSb_3$ — ***Sinn-wen Chen***, *Zi-yang Huang, Yang-yuan Chen*

Paper 199i: Theoretical Study of a High-Performance Thermoelectric Material: Stanene — ***Pabitra Choudhury***, *Charles Griego*

Paper 199j: Revealing the Enigmatic Interfacial Layer of Core/Shell Quantum Dots — ***Ajay Singh***, *Jennifer Hollingsworth*

Paper 199k: Spatial Manipulation of Thermal Flux Profiles Using Nanostructure Boundaries — ***Abhinav Malhotra***, *Martin Maldovan*

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(200) Poster Session: Materials Engineering & Sciences (08F — Composite Materials)
Monday, Oct 30, 3:15 PM
MCC, Exhibit Hall B

Megan L. Robertson, Chair
Zhengtang Luo, Co-Chair
Jeffrey Rimer, Co-Chair

Sponsored by:
Materials Engineering and Sciences Division

Paper 200a: Magnetic Polymer Nano-Composites for Giant Magnetoresistance and Electromagnetic Shielding — ***Jiang Guo***, *Alexandra Galaska, Brian J. Edwards, Bamin Khomami, Zhanhu Guo*

Paper 200b: Constructing Ternary Conductive Polymer Composites with Cocontinuous Polymer Blends and Interfacial Graphene Nanoplatelets — ***Yangming Kou***, *Lian Bai, Xiang Cheng, Christopher W. Macosko*

Paper 200c: The Influence of Interfacial Graphene on the Morphological, Electrical and Mechanical Properties of Co-Continuous Polymer Blends — ***Catherine Esnaashari***, *Lian Bai, Christopher W. Macosko, Xiang Cheng*

Paper 200d: The Fabrication and Application of Composite Graphene Oxide Films — *Jiaxin Shen, Yafei Feng, Cunliang Ma,* ***Yidong Liu***, *Yong Min*

Paper 200e: Mechanically Stable Thermally Crosslinked Poly(acrylic acid)/ Reduced Graphene Oxide Aerogels — *Heonjoo Ha,* ***Han Xiao***, *Kadhiravan Shanmuganathan, Christopher J. Ellison*

Paper 200f: Ionophore-Decorated Magnetic Graphene Oxide as a Composite Adsorbent Material for Heavy Metal Ion Sequestration — ***Khino J. Parohinog***, *Grace M. Nisola, Wook-Jin Chung*

Paper 200g: Synthesis of Thermoresponsive Polymer/Fe_3O_4 Nanoparticle Composite and Its Application — ***Risako Sakai***, *Junichi Ida, Tatsushi Matsuyama*

Paper 200h: High-Performance, Ambient Phase Change Thermal Diodes for Energy Applications — ***Anton Cottrill***, *Song Wang, Albert Tianxiang Liu, Yuichiro Kunai, Michael S. Strano*

Paper 200i: A Study on the Preparation and Properties of Polymer Composites Using Amino-Functionalized Microcrystalline Cellulose (MCC) as a Filler Material — ***KiRyong Ha***, *Hanna Kim, Yeokyung Yang, KiSeob Hwang, Kwang-Hee Lim*

Paper 200j: Electrically Conductive Films Made of Polythiophene and Fibrillated Wood Particles — ***Islam Hafez***, *Han-Seung Yang, William T. Y. Tze*

Paper 200k: PEG-Coated Fe_3O_4@MIL-100 (Fe): A Potential Carrier for Doxorubicin Delivery — ***Abhik Bhattacharjee***, *Sasidhar Gumma, Mihir K. Purkait*

Paper 200l: Effect of Different Carbon Additives on Structure of Magnesium Composites for Hydrogen Storage — ***Yeboah Martin Luther***

Paper 200m: Four Reversible and Reconfigurable Structures for Three-Phase Emulsions: Extended Morphologies and Applications — ***Xuehui Ge***

Paper 200n: Low Loading of Grafted Thermoplastic Polystyrene Strengthened and Toughened Transparent Epoxy Composites — ***Chao Ma***, *Hongbo Gu*

Paper 200o: Preparation of Modified Graphene Oxide–Containing Styrene Masterbatches for Thermosetting Resin Composite — ***Siyao He***, *Yuqiang Qian, Kunwei Liu, Chris Macosko, Andreas Stein*

Paper 200p: Smart Windows Enabled by Buckling Instabilities in Periodic Composite Films — ***Peng Jiang***, *Zhuxiao Gu*

Paper 200q: Magnetic Polymer Nanocomposites for Electromagnetic Interference Shielding — ***Jiang Guo***, *Alexandra Galaska, Suying Wei, Brian J. Edwards, Bamin Khomami, Zhanhu Guo*

(201) Poster Session: Nanoscale Science and Engineering
Monday, Oct 30, 3:15 PM
MCC, Exhibit Hall B

Reginald E. Rogers Jr., Chair
Micah Green, Co-Chair
Ardemis A. Boghossian, Co-Chair
Daniel S. Charles, Co-Chair

Sponsored by:
Nanoscale Science and Engineering Forum

Paper 201a: IrO_2 Nanopore MEA for Highly Efficient Oxygen Evolution Electrocatalyst in SPE — ***Zhuoxin Lu***, *Yan Shi, Changfeng Yan*

Paper 201b: Synthesis and Electrochemical Characterization of Ordered Pt Nanopattern Catalysts Through Self-Assembling Block Copolymer — *Yuan Guan, Zhi-da Wang,* ***Changfeng Yan***

Paper 201d: Carbonic Anhydrase-Based Nanocomposites for CO_2 Conversion and Utilization — ***Han Sol Kim***, *Sung-Gil Hong, Jungbae Kim*

Paper 201f: Immobilization and Stabilization of Acylase via Nanobiocatalytic Approach for Enzymatic Antifouling — ***Jahyun Nam***, *Byoungsoo Lee, Kyung-Min Yeon, Jinwoo Lee, Jungbae Kim*

Paper 201g: Promoter Effect of Alklyamine-Functionalized Silica on Gold Nanoparticle–Catalyzed Hydroamination Reactions — ***Trent R. Graham***, *Steven R. Saunders*

Paper 201h: The Effect of Microenvironment on the Catalytic Ability of Multifunctional Nanoreactors — ***Andrew Harrison***, *Tien Vuong, Matthew Nguyen, Christina Tang*

Paper 201i: Evaluation of the Cancer-Preventive Effect of Resveratrol-Loaded Nanoparticles on the Formation of Lung Tumor Spheroids — ***Elisa A. Torrico-Guzmán***, *Samantha A. Meenach*

Paper 201j: Preparation of Monodisperse, Supported Nanoparticles with Switchable Surfactants — ***Kristin Bryant***, *Gasim Ibrahim, Steven R. Saunders*

Paper 201k: Metal Ion–Triggered Assembly of Peptide-Drug Conjugates — ***Han Wang***, *Hao Su, Honggang Cui*

Paper 201l: Crystal Structure of Coalescing CdSe Nanoparticles by Molecular Dynamics Simulations — ***Eirini Goudeli***, *Stefano Lazzari*

Paper 201m: Hybrid Inorganic Nanosheets and Metal-Organic Frameworks for Efficient Photocatalytic Water Splitting — ***Hyunuk Kim***, *Tae Woo Kim*

Paper 201o: Solvent Engineering of Molybdenum Disulfide Electro-Catalysts for Hydrogen Evolution — ***Isaiah Woodson***, *Venkata Vasiraju, Delaina A. Amos, Gautam Gupta*

Paper 201q: 3D Graphene/Platinum Nanowire Hybrid Composite Electrodes via Electrostatic Self-Assembly for Supercapacitor Applications — ***Jenny Wang***, *Stephen Winter, F. John Burpo, Enoch Nagelli*

Paper 201r: Polyelectrolyte-Wrapped Carbon Nanotubes/Platinum Nanowire Hybrid Composite Electrodes via Electrostatic Self-Assembly for Energy Storage and Conversion Applications — ***Dade Mortimer***, *An Vu, MAJ Stephen Winter, COL F. John Burpo, Enoch Nagelli*

Paper 201s: Dissolution Behavior of Thermally Grown SiO_2 — ***Young Hee Yoon***, *Yoon Kyeung Lee, John A. Rogers*

Paper 201t: Laser-Activated Tissue-Integrating Sutures for Rapid Closure of Soft Tissue — ***Russell Urie***, *Deepanjan Ghosh, Tanner Flake, Jerry Crum, Jacquelyn Kilbourne, Kaushal Rege*

Paper 201u: Bio-Templated Nanoparticle Synthesis: Fundamental and Theoretical Studies — ***Abdollah Mosleh***, *Rita Tejada Vaprio, Hayden Hairston, Bob Beitle, Mahmoud Moradi, Lauren F. Greenlee, Nicholas Bedford*

Paper 201v: TiO_2 Nanotubes: Design and Structure Optimization — ***Anthony Videckis,*** *Jevin Meyerink, Grant Crawford*

Paper 201w: Dispersion Behavior of DNA-Wrapped Carbon Nanotubes Under Different Environments — ***Niyousha Mohammadshafie***, *Geyou Ao*

Paper 201x: 3D Graphene-Carbon Nanotube-Fe_3O_4 Anode for High-Performance Li-Ion Batteries — ***Victoria Zane***, *Huan Wang, Placidus B. Amama*

Paper 201y: Fabrication of a Microwell Array for High-Throughput Screening and Discovery of Bacterial Interactions — ***Logan McGinley***, *Niloy Barua, Ryan Hansen*

Paper 201z: Evaluation of Operational Variables in the Degradation of Orange II Using Iron Nanoparticles Supported on Fique Fibers — ***Karen Giovanna Bastidas Gómez***, *Hugo Ricardo Zea Ramírez, Cesar Augusto Sierra Avila*

Paper 201aa: Aerosol Synthesis of Highly Porous Carbon with Nanosheet Morphology for Improved Ionic Sorption Capacitance — ***Kyeong Youl Jung,*** *Byeong Ho Min*

Paper 201ab: Preparation of Carbon-MnO_2 Nanocomposites by Chemical Redox Deposition for Application to Asymmetric Electrochemical Capacitor — ***Sang Mun Jeong***, *En Mei Jin*

Paper 201ac: Two-Dimensional Cobalt/N-Doped Carbon Hybrid Structure Derived from Metal-Organic Frameworks as Efficient Electrocatalysts for Hydrogen Evolution — ***Tan Huang***

Paper 201ad: Morphological Control of Li_3VO_4 via Solvothermal Synthesis and Electrochemical Performance for Lithium-Ion Batteries — ***Guang Yang***

Paper 201ae: Detailed Characterization and Fabrication of 3D-Printed Graphene/Polymer Structures For Heterojunction Devices with MoS2 and Other 2D Nanomaterials — *Deisy Arrington, Dylan Lynch,* ***Vikas Berry***

Paper 201af: Photovoltaic and Spectral Response of WS_2/Silicon Heterojunctions — *Sanjay Behura, Kai-Chih Chang, Yu Wen, Rousan Debbarma, Phong Nguyen, Songwei Che, Shikai Deng, Michael Seacrist,* ***Vikas Berry***

Paper 201ag: All-CVD Direct Growth of Large-Scale Graphene and Hexagonal Boron Nitride Heterostructures — ***Sanjay Behura***, *Phong Nguyen, Chen Wang, Songwei Che, Rousan Debbarma, Michael R. Seacrist, Vikas Berry*

Paper 201ah: A Novel Technique for Rapidly Synthesizing Small Unilamellar Liposomes with High Encapsulation Efficiencies — ***Steven Roberts***, *Nitin Agrawal*

Paper 201ai: Magnetization Dynamics and Energy Dissipation of Interacting Magnetic Nanoparticles in Dynamic Magnetic Fields — ***Zhiyuan Zhao***, *Carlos Rinaldi*

Paper 301f: Titanium Nitride Nanotube As Effective Cathode Materials for Lithium Sulfur Batteries — ***Wenduo Zeng***, *Mark Cheng, Simon Ng*

(202) Poster Session: Novel Products from Forest and Plant Biomass
Monday, Oct 30, 3:15 PM
MCC, Exhibit Hall B

Shri Ramaswamy, Chair
Shijie Liu, Co-Chair

Sponsored by:
Forest and Plant Bioproducts Division

Paper 202a: Rapid and Near-Complete Dissolution of Wood Lignin at ≤ 80°C Using a Recyclable Acid Hydrotrope for Sustainable Production of High-Value Building Blocks — ***J. Y. Zhu***, *Liheng Chen, Huiyang Bian, Ruchun Wu, Shiyu Fu*

Paper 202b: Tuning the Physicochemical Properties of Biochar Derived from Ashe Juniper by Vacuum Pressure and Temperature — *Julius Choi,* ***Sergio Capareda***

Paper 202c: Biochar: A Sustainable Fuel Source — ***Christopher Ellithorpe***, *Amanda Simson, Eddie Luzik, Morgan Nivison, Micah Fertig*

Paper 202d: Renewable Transportation Biofuel Converted from Wet Biowaste via Hydrothermal Liquefaction — ***Wan-Ting Chen***, *Yuanhui Zhang, Timothy Lee, Zhenwei Wu, Chia-Fon Lee, B. K. Sharma*

Paper 202e: Co-Gasification of Woody Biomass and Chicken Manure — *Wei Cheng Ng, Siming You, Ran Ling, Karina Yew-Hoong Gin, Yanjun Dai,* ***Chi-Hwa Wang***

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(203) Poster Session: Pharmaceutical
Monday, Oct 30, 3:15 PM
MCC, Exhibit Hall B

Zoltan K. Nagy, Chair

Sponsored by:
Pharmaceutical Discovery, Development and Manufacturing Forum

Paper 203a: Large-Scale Synthesis of Dihydrostreptomycin via Hydrogenation of Streptomycin in a Membrane Dispersion Microreactor — ***Siting Xia***, *Xifeng Ding,* ***Yujun Wang***, *Guangsheng Luo*

Paper 203c: Direct Comparison Between Batch Bulk Mixing and Continuous Millifluidics in the Synthesis of Amorphous Drug Nanoparticles — *Kunn Hadinoto,* ***Jia Wei Chew***

Paper 203d: Novel Method of Evaluating Liquid Absorption with Intra-Particle Pore of Pharmaceutical Porous Materials Using a Capillary Rise Method — ***Takuma Oba***, *Yasutomi Kato, Ryoichi Sonoda, Kohei Tahara, Yoshiaki Kawashima, Hirofumi Takeuchi*

Paper 203e: Evaluation of Experimental Methods for Solubility Determination of Carbamazepine in Ethanol for Cooling Crystallization Process Design — ***Wei-Lee Wu***, *David A. Acevedo, Xiaochuan Yang, Thomas O'Connor, Celia N. Cruz*

Paper 203f: Continuous Solvent Exchange Washing of Pharmaceutical Intermediates — ***Manuel Kreimer***, *Isabella Aigner, Stephan Sacher, Markus Krumme, Thomas Mannschott, Peter van der Wel, Albert Kaptein, Johannes G. Khinast*

Paper 203g: Design and Characterization of Fast-Release Clofazimine Nanoparticles to Improve Bioavailability — ***Yingyue Zhang***, *Jie Feng, Simon A. McManus, Hoang D. Lu, Kurt D. Ristroph, Robert K. Prud'homme*

Paper 203h: Design of Efficient Metal Nanocatalysts for Continuous Synthesis of Drug Substances via Cross-Coupling Reactions — ***Andishaeh Dadgar***, *Farshid Mohammadparast, Marimuthu Andiappan*

Paper 203i: Downstream Processing of Extrudates: Polymer Platform Development for Hot-Melt Extrusion/Tableting via In-Line Monitoring of Compaction Properties — ***Wouter Grymonpré***, *Valérie Vanhoorne, Thomas De Beer, Jean Paul Remon, Chris Vervaet*

Paper 203j: Virtual High-Throughput Screening Pipeline: Size and Classification Distribution Effects on Experimentally Validated Hit Rates — ***Jonathan J. Chen***, *Donald P. Visco Jr., Lyndsey Schmucker*

Paper 203k: RNAi Screening of Endocytic Uptake Mechanisms in Polymer-Mediated Gene Delivery — ***Landon A. Mott***, *Daniel Pack*

Paper 203l: PAT on Oscillatory Systems: Monitor and Control Continuous Crystallization with Fourier Transform Infrared (FTIR) Spectrometer — ***Claire Yiqing Liu***, *Jonathon Speed, Dan Wood, Alastair Barton, Paul Firth, Zoltan K. Nagy*

Paper 203m: Continuous Manufacturing of Oral Disintegrating Films: A Quality-by-Design Approach — ***Sonal Mazumder***, *Xiaoming Xu, Cassandra Taylor, Nima Yazdanpanah, Thomas O'Connor, Ashraf Muhammad, Celia N. Cruz, Naresh Pavurala*

Paper 203n: Controlled Delivery of Fluorophores from 3D Two-Photon Photolithographic Printed Poly(Ethylene Glycol) Methacrylate Scaffolds — ***Anh-Vu Do,*** *Kristin Worthington, Budd A. Tucker, Aliasger K. Salem*

Paper 203o: Controlled and Sequential Delivery of Fluorophores from 3D-Printed Alginate-PLGA Tubes — ***Anh-Vu Do***, *Adil Akkouch, Brian J. Green, Ibrahim Ozbolat, Aliasger K. Salem*

Paper 203p: The Pressurized-Synthetic Methodology for Solubility Determination at Elevated Temperatures, with Application to Paracetamol in Pure Solvents — *Brian de Souza,* ***Leila Keshavarz***, *Patrick Frawley*

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(204) Poster Session: Thermodynamics and Transport Properties (Area 1A)
Monday, Oct 30, 3:15 PM
MCC, Exhibit Hall B

Andrew Paluch, Chair

Sponsored by:
Thermodynamics and Transport Properties

■ PHASE EQUILIBRIA

Paper 204a: Prediction of Vapor Pressure and Critical Properties for Non-Electrolyte Organic Compounds from PR+COSMOSAC EOS — *Chien-Yi Li,* ***Chieh-Ming Hsieh***

Paper 204b: Volumetric Properties of Saccharide in Aqueous Ionic Liquid Mixtures at Different Temperatures — *Natalia D. F. Val, Heloisa E. Hoga,* ***Ricardo B. Torres***

Paper 204c: Density and Derived Properties of Binary Mixtures Containing {Dimethyl Carbonate (DMC) + 1-Propanol} at T = (288.15 to 308.15) K and at P = (0.1 to 40) mpa — *Gustavo V. Olivieri,* ***Ricardo B. Torres***

Paper 204d: Triangular-Well Fluid Equation of State: Extension to Mixtures — ***Luis A. Galicia-Luna***, *Jaime A. Riera-Ortiz, Felix F. Betancourt-Cárdenas*

Paper 204e: A SAFT Equation of State Based on Triangular-Well Fluid Potential — ***Luis A. Galicia-Luna***, *Alfredo Pimentel-Rodas, Jaime A. Riera-Ortiz, Jose M. Rosete-Barreto*

Paper 204f: Experimental Determination of Phase Equilibria of Clathrate Hydrates of Mixture Water + Hexane + Decane + Carbon Dioxide and Semi-Clathrates Hydrates of Mixture Water + Thermodynamic Promoter + Hexane + Decane + Carbon Dioxide — *Angel M. Notario-López Sr., Pedro Esquivel-Mora,* ***Luis A. Galicia-Luna***

Paper 204g: Modelling the Solubility of Naphthalene and Phenanthrene in Binary and Ternary Systems Containing Carbon Dioxide — ***Francisco Javier Verónico Sánchez***, *Miguel Gonzalo Arenas Quevedo, Octavio Elizalde-Solis*

Paper 204h: Molecular-Inspired Parameters Concealed in the Van Der Waals Attractive Force Revealed by First Principles, Statistical Mechanics and Perturbation Methods — ***Akanni S. Lawal***

Paper 204i: Solid-Liquid Equilibria for Selected Binary Mixtures Containing Diphenyl Carbonate — ***Hiroyuki Matsuda***, *Yuki Ohashi, Kiyofumi Kurihara, Katsumi Tochigi*

■ ADSORPTION AND INTERFACES

Paper 204j: Thermophysical Suitability of Terphenyl for Hydrogen Storage — ***Jonas Obermeier***, *Yannick Werner, Ferdinand Heusinger, Michael Geißelbrecht, Patrick Preuster, Peter Wasserscheid,* ***Wolfgang Arlt***, *Karsten Müller*

Paper 204k: Atomic-Level Mechanistic Insights into Monolayer hBN Growth from Reactive Molecular Dynamics Simulations for Catalysis Applications — ***Bin Liu***, *Song Liu, Mingxia Zhou, James H. Edgar*

Paper 204l: Differential Retention and Release of CO_2 and CH_4 in Kerogen Nanopores: Implications for Gas Extraction and Carbon Sequestration — ***Tuan Ho***, *Louise J. Criscenti, Yifeng Wang*

■ BIOMOLECULAR SYSTEMS

Paper 204m: Investigation of Electronic Properties of Imidazolium-Based Ionic Liquids in the Presence of Iron Porphyrins for Understanding Their Biodegradability — ***Atiya Banerjee***, *Jindal K. Shah*

Paper 204n: Capturing the Membrane-Triggered Conformational Transition for Pore-Forming Cytolysin (ClyA) Using Structure-Based Models — *Hemanth Giri Rao V. V., Rajat Desikan, Shachi Gosavi,* ***K. G. Ayappa***

Paper 204o: Solid Form Transformation of Disodium Guanosine 5′-Monophosphate: Thermodynamic Perspective — ***Qiao Chen***, *Fengxia Zou, PengPeng Yang, Jinglan Wu, Wei Zhuang, Hanjie Ying*

■ TRANSPORT PROPERTIES

Paper 204p: Estimation of Kinematic Viscosity for CO_2-Expanded Liquids by ASOG-VISCO Method — *Toshitaka Funazukuri, Hiroyuki Matsuda, Kiyofumi Kurihara,* ***Katsumi Tochigi***, *V. K. Rattan*

Paper 204q: On the Kac-Based Collision Models from Simplified Bernoulli till Its Intelligent Variants — ***Bijan Goshayeshi***

Paper 204r: Viscosity and Derived Properties of Binary Mixture Containing Acetonitrile + 1-Propanol at Different Temperatures and Atmospheric Pressures — *Christian A. T. Campos, Heloisa E. Hoga,* ***Ricardo B. Torres***

Paper 204s: Volumetric, Acoustic and Viscometric Properties of Binary Mixture of (n-butylammonium methanoate + 1-propanol) at Different Temperatures — *Robert L. Fernandes, Heloisa E. Hoga,* ***Ricardo B. Torres***

Paper 204t: Measurement of Diffusion Coefficients of Chromium(III) Acetylacetonate in Supercritical Carbon Dioxide at High Temperatures — ***Minoru Yamamoto***, *Junichi Sakabe, Minori Taguchi, Toshitaka Funazukuri*

Paper 204u: Simultaneous Determinations of Dynamic Viscosity and Density of Several Alcohols Using Straight and Coil Capillary Viscometers at Temperatures Between (313–353) K and Pressures up to 30 mpa — *Alfredo Pimentel-Rodas,* ***Luis A. Galicia-Luna***, *Jose J. Castro-Arellano*

Paper 204v: Analysis of High-Speed Rotating Flow Inside Gas Centrifuge Casing — ***Sahadev Pradhan***

Paper 204w: DSMC Simulations of High–Mach Number Taylor-Couette Flow — ***Sahadev Pradhan***

Paper 204x: Viscosity Prediction of the Carbon Dioxide–Loaded Aqueous Solutions of Alkanolamines: Thermodynamic Approach — ***Naser S. Matin***, *Joseph E. Remias, Kunlei Liu*

Paper 204y: A Computational Study on the Transport of Actives Through Skin Layers — ***Kishore Gajula,*** *Rakesh Gupta, Dwadasi Balarama Sridhar, Beena Rai*

(205) Advanced Oxidation Processes II
Monday, Oct 30, 3:15 PM
MCC, 102F

Robert W. Peters, Chair
Mohammed Mostafa, Co-Chair
Tapas K. Das, Co-Chair
Selma Mededovic Thagard, Co-Chair

Sponsored by: Water

3:15 Paper 205a: Optimizing Drinking Water Disinfection: Balancing Corrosion, Byproduct Formation, and Pathogen Removal — ***Margaret M. Reuter***, *Christian M. Lastoskie*

3:40 Paper 205b: Enhanced Oxidation of Toxic Organic Pollutants by Ferrate(VI) and Its Modifications in Aqueous Solution — *Kyriakos Manoli, George Nakhla, Virender K. Sharma,* ***Ajay K. Ray***

4:05 Paper 205c: Cyanide Recovery from Barren Solution Using UV Photodissociation and Gas-Filled Membrane Technology — ***Kashinath Banerjee***, *Herve Buisson, Tapas K. Das*

4:30 Paper 205d: Removal of Phenol from Wastewater of Petroleum Refinery by Using Advanced Oxidation Process — ***Ghanim M. Alwan Sr.***, *Mohmmed Abid Sr., Lamyaa Abdulrihda*

(206) Advances in Fluid-Particle Separations
Monday, Oct 30, 3:15 PM
MCC, M100G

Isaac Gamwo, Chair
Seyi Odueyungbo, Co-Chair

Sponsored by: Fluid-Particle Separations

3:15 Paper 206a: Scale-Up and Optimization of Filtration Processes: Small-Scale Pressure Filtration to Centrifugal Filtration — ***Niall Mitchell***, *Christopher S. Polster, Christopher L. Burcham, Kevin Girard, Sean Bermingham*

3:33 Paper 206b: Steady-State Elutriation of Fines from Binary Particle Mixtures in Bubbling Fluidized Cold Flow Model — ***Nicholas Hillen***, *Ronald W. Breault, Steven Rowan, Justin Weber*

3:51 Paper 206c: Sustainable Fractionation of Plant-Derived Proteins with Pneumatic Tribo-Electrostatic Separation — ***Solmaz Tabtabaei***, *Amin R. Rajabzadeh, Raymond L. Legge*

4:09 Paper 206d: Particle Image Velocimetry (PIV): An Important Tool for Understanding the Fluid Dynamics of Magnetically Responsive Membranes — ***Arijit Sengupta***, *M. G. Jebur, Ranil Wickramasinghe, Xianghong Qian*

4:27 Paper 206e: Overview of Real-Time Monitoring Techniques for Drop Size Distributions in Research and Industrial Applications — ***Sebastian Maaß***, *Jörn Emmerich, Matthias Kraume*

4:45 Paper 206f: Sedimentation of Agglomerates Consisting of Polydisperse Nanoparticles — *Anastasia Spyrogianni, Katerina S. Karadima, Eirini Goudeli, Vlasis G. Mavrantzas,* ***Sotiris E. Pratsinis***

5:03 Paper 206g: Numerical Study on the Separation Characteristics and Kinematic Behavior of Particles in a Hydrocyclone — ***Yanxia Xu,*** *Jianguo Yu*

5:21 Paper 206h: Evaluation of the Efficacy and Mechanism of Cactus (*Opuntia ficus-indica*) as a Natural Coagulant for Pre-Treatment of Oil Sand Process–Affected Water — ***Manisha Choudhary***, *Madhumita Ray, Sudarsan Neogi*

(207) Applied Environmental Catalysis II
Monday, Oct 30, 3:15 PM
MCC, L100B

Eleni A. Kyriakidou, Chair
Di Wang, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

3:15 Paper 207a: The Role of Oxygen Vacancies of CeO_2 Supported Catalyst on Catalytic Performance of the CO_2 to CO — ***Sheng-Chiang Yang***, *Wei-Nien Su, Simon H. Pang, Taylor Sulmonetti, Bing Joe Hwang, Christopher W. Jones*

3:33 Paper 582cj: CO, C_2H_2, and C_3H_6 Oxidation on Pd/Ceria-Zirconia/Al_2O_3 Three-Way Catalysts: Experiments and Modeling — ***Wendy Lang***, *Michael P. Harold, Yisun Cheng, Carolyn Hubbard, Paul Laing*

3:51 Paper 207c: One-Step Synthesis of Transition Metal–Doped Titanium Dioxide Catalysts for Oxygen Removal — ***Sungyoon Jung***, *Pratim Biswas*

4:09 Paper 207d: Carboxylation of Propylene Oxide to Propylene Carbonate — ***Pallavi Bobba***, *Bala Subramaniam, R. V. Chaudhari*

4:27 Paper 207e: Improving the Performance of Sn-Promoted Ni/Al_2O_3 Catalysts for the Dry Reforming of Methane — *Thomas Stroud, Estelle Le Saché, Tristan Smith, Harvey Arellano-Garcia,* ***Tomás Ramirez-Reina***

4:45 Paper 207f: Advanced Ni-CeO_2/Al_2O_3 Nanocatalysts for Chemical CO_2 Recycling — *Tristan Smith, Estelle Le Saché, Thomas Stroud, Harvey Arellano-Garcia,* ***Tomás Ramirez-Reina***

5:03 Paper 207g: Two-Step Selective Bromination of Thiophenic Compounds for Gasoline Desulfurization Under Mild Conditions — *Guang Miao, Cuiting Yang, Zhong Li,* ***Jing Xiao***

5:21 Paper 207h: Improvement of Low-Temperature Activity for CO Oxidation on Ceria Catalyst by Transition Metal Substitution — ***HyungJun Kim***, *Kyung-Jong Noh, Geonhee Lee, Jeong Woo Han*

(208) Area Plenary: Adsorption and Ion Exchange II
Monday, Oct 30, 3:15 PM
MCC, M100E

Stefano Brandani, Chair
Matthias Thommes, Co-Chair

Sponsored by: Adsorption and Ion Exchange

3:15 Paper 208a: Thermogravimetric and Breakthrough Studies on the Adsorption Reversibility of SO_2, NO_2 and NO on Type A and X Zeolites — ***Armin D. Ebner***, *Marjorie A. Nicholson, Peter A. Fairchild, James A. Ritter*

3:35 Paper 208b: The Correct Use of the Ideal Adsorbed Solution Theory for High-Pressure Systems — ***Stefano Brandani***

3:55 Paper 208c: Mapping the Limitations of Breakthrough Analysis in Fixed-Bed Adsorption — ***James C. Knox***, *Armin D. Ebner, James A. Ritter*

4:15 Paper 208d: Calculation of the Isosteric Enthalpy of Adsorption in Monte Carlo Molecular Simulation: New Equations Addressing Bulk-Phase Nonideality and Isosteres of Total Adsorption — ***Daniel W. Siderius***, *Nathan A. Mahynski, Vincent K. Shen*

4:35 Paper 208e: Compressibility of Argon Confined in Nanopores: Effect of the Pore Geometry — *Christopher D. Dobrzanski,* ***Gennady Gor***

4:55 Paper 208f: Ligand-Assisted Displacement Chromatography for Rare Earth Elements Separations — ***Hoon Choi***, *David M. Harvey, Lei Ling, Nien-Hwa Linda Wang*

5:15 Paper 208g: Adsorption Studies of Tryptophan in a BSA-Coated Surface in Semi-Batch Fractionation and Microchannel — ***Avinash Sahu,*** *Akshay Govindrajan, S. Pushpavanam*

(209) Area Plenary: Sustainability and the RAPID (Rapid Advancement in Process Intensification Deployment) Manufacturing Institute (Invited Talks)
Monday, Oct 30, 3:15 PM
MCC, 101D

Lindsay Soh, Chair
Fengqi You, Co-Chair

Sponsored by: General

3:15 Paper 209a: Rapid Advancement in Process Intensification Deployment (RAPID): US Efforts to Establish a Modular Chemical Process Intensification Manufacturing Institute — ***Karen Fletcher***

3:40 Paper 209b: Modeling and Simulation: A Key Component in Enabling Process Intensification — ***David Sholl***, *Efstratios N. Pistikopoulos*

4:05 Paper 209c: Modeling and Simulation Challenges for Process Intensification — ***Efstratios N. Pistikopoulos***, *David Sholl, M. M. Faruque Hasan, Salih E. Demirel, Yuhe Tian*

4:30 Paper 209d: The Sustainable Synthesis-Design-Intensification of Chemical and Biochemical Processes — ***Rafiqul Gani***, *Deenesh K. Babi, Maria-Ona Bertran, Rebecca Frauzem, Nipun Garg*

4:55 Paper 209e: Democratizing Energy Technology — ***Dane Boysen***

5:20 Panel Discussion

(210) Best Practices in Pilot Plants
Monday, Oct 30, 3:15 PM
MCC, 102C

Oliver Orrell, Chair
Martin Gomez Osorio, Co-Chair

Sponsored by: Pilot Plants

3:15 Paper 210a: "We Don't Expect It to Be a Problem": Best Practices in Pilot Plant Start-Up — ***Richard Palluzi***

3:40 Paper 210b: Optimal Steady-State and Dynamic Design of Experiments in Pilot Plants for CO_2 Capture — ***Joshua C. Morgan***, *Anderson Soares Chinen, Christine Anderson-Cook, K. Sham Bhat, Benjamin P. Omell, Ryan Hughes, Goutham Kotamreddy, Michael Matuszewski, Charles Tong, David C. Miller, Justin H. Anthony, Chiranjib Saha, Debangsu Bhattacharyya*

4:05 Paper 210c: Demonstration of a Commercial-Scale Circulating Fluidized-Bed Gasifier for Industrial Fuel Gas — ***ZhiPing Zhu***

4:30 Paper 210d: Collaborative Bioprocess Development and Piloting at DOE's Berkeley National Lab ABPDU for Industrial Chemicals, Fuels, Materials, and Food Ingredient Production — ***Todd Pray***, *Deepti Tanjore, Ning Sun, Akash Narani*

4:55 Paper 210e: Cold Model Study of Hydro-Dynamic Parameters Affecting the Performance of Re-Circulating Fluidized Bed — ***Nitin Lokachari***, *Raman Sharma, Sachin Tomar*

5:20 Paper 210f: Troubleshooting Anomalous Behaviour in a Solid-State Reaction Process — ***Eric Grolman,*** *Micaela Caramellino*

(211) Catalytic Processing of Fossil and Biorenewable Feedstocks III: Alcohols and Polyols
Monday, Oct 30, 3:15 PM
MCC, L100C

Ana C. Alba-Rubio, Chair
Thomas J. Schwartz, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

3:15 Paper 211a: Catalytic Ethanol Conversion to 1,3-Butadiene on MgO/SiO_2: Reactive Catalyst Surface Structure and Reaction Mechanisms — *William Taifan, George Xu Yan, Tomas Bucko,* ***Jonas Baltrusaitis***

3:35 Paper 211b: Characterization of the Active Site and Mechanism for 1,6-Hexanediol Production from Tetrahydrofuran-Dimethanol over Pt-Based Catalysts — ***Samuel P. Burt***, *Jiayue He, James A. Dumesic, George W. Huber, Ive Hermans*

3:55 Paper 211c: Mechanism and Kinetics of 1-Dodecanol Etherification and Dehydration over Tungstated Zirconia — ***Julie Rorrer***, *Dean Toste, Alexis T. Bell*

4:15 Paper 211d: A Three-Step Catalytic Pathway for the Scalable Production of 1,5-Pentanediol from Biomass-Derived Tetrahydrofurfuryl Alcohol — ***Kevin J. Barnett***, *Zachary Brentzel, Kefeng Huang, Ling Li, Guozhu Liu, Christos T. Maravelias, James A. Dumesic, George W. Huber*

4:35 Paper 211e: Continuous Condensed-Phase Conversion of Ethanol to Higher Alcohols over Bimetallic Catalysts — ***Iman Nezam***, *Dennis J. Miller*

4:55 Paper 211f: The Effects of Metal-Acid Site Proximity on Bifunctional Isomerization of Alkanes and Deoxygenation of Alcohols — ***Gina Noh***, *Yongchun Hong, Weiting Yu, Enrique Iglesia*

5:15 Paper 211g: The Influence of Solvent on Acid-Catalyzed Dehydration of Model Polyols — ***Chotitath Sanpitakseree***, *Max A. Mellmer, Benginur Demir, Peng Bai, Kaiwen Ma, Matthew Neurock, James A. Dumesic*

(212) Chemical-Looping Processes II
Monday, Oct 30, 3:15 PM
MCC, 103A

Kevin Whitty, Chair
JoAnn S. Lighty, Co-Chair
Shwetha Ramkumar, Co-Chair
Samuel Bayham, Co-Chair

Sponsored by: Innovations of Green Process Engineering for Sustainable Energy and Environment

3:15 Paper 212a: Hydrogen Production from Heavy Fraction of Bio-Oil Based on Iron-Based Chemical-Looping System with Carbon Capture — ***Lijun Heng***, *Huiyan Zhang, Rui Xiao, Mengmeng Zhou*

3:36 Paper 212b: Chemical-Looping Gasification with Red Mud as the Oxygen Carrier and Catalyst for Hydrogen-Rich Syngas Production — ***Jinhua Bao***, *Liangyong Chen, Liang Kong, Zhen Fan, Heather Nikolic, Kunlei Liu*

3:57 Paper 212c: Updates on the Operation of NETL's 50-kW Chemical-Looping Combustion Test Facility — ***Samuel Bayham***, *Douglas Straub, Justin Weber*

4:19 Paper 212d: Assessment of Looping Combustion and Gasification of Carbon (CarboLoop) in a Twin Fluidized-Bed Reactor — *Antonio Coppola,* ***Piero Salatino***, *Osvalda Senneca*

4:40 Paper 212e: Super-Dry Reforming of CH_4 — ***Lukas Buelens***, *Vladimir V. Galvita, Hilde Poelman, Guy B. Marin*

5:01 Paper 212f: Efficiency Evaluation of Combined-Cycle Power Plants Integrated with Fixed-Bed Chemical-Looping Combustion Reactors — ***Chen Chen***, *George M. Bollas*

5:23 Paper 212g: Fate of Sulfur in Coal-Direct Chemical-Looping Systems — ***Cheng Chung***, *Yaswanth Pottimurthy, Mingyuan Xu, Tien-Lin Hsieh, Dikai Xu, Yitao Zhang, Yu-Yen Chen, Pengfei He, Marshall Pickarts, Liang-Shih Fan, Andrew Tong*

TECHNICAL SESSIONS 2017

(213) ChE Potpourri: Beer and Thermodynamics
Monday, Oct 30, 3:15 PM
MCC, 205D

Anju Gupta, Co-Chair
Donald P. Visco Jr., Co-Chair

Sponsored by:
Undergraduate Education

3:15 Paper 213a: Developing Chemical Engineering Acumen by Brewing Kicking Mule Beer — *Matthew Armstrong,* ***Joshua White****, Geoffrey Bull, Jesse Hudgins*

3:39 Paper 213b: Beer Experiments: A Hopping Success — ***Claire F. Komives****, Corey Lapeyri, Alexis Venegas, Diego Marquez, Joseph Pesek*

4:03 Short Topic Transition

4:09 Paper 213c: Why Is the Mustard in the Fridge? A Fun Assignment on the Thermodynamics of Food Safety — ***Margot Vigeant***

4:33 Paper 213d: Improving Conceptual Knowledge and Retention in Introduction to Engineering Thermodynamics — ***Rachel Morrish***

4:57 Paper 213e: Tax Revenue Laffer Curve from Thermodynamics Perspective — ***Min Huang***

5:21 Paper 213f: The Art of the Game: Infusing Thermodynamics Learning with Classic Household Games — ***Reginald E. Rogers Jr.***

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(214) Continuous Crystallization Processes
Monday, Oct 30, 3:15 PM
MCC, M100J

Christopher L. Burcham, Chair
Nima Yazdanpanah, Co-Chair

Sponsored by:
Crystallization and Evaporation

3:15 Welcoming Remarks

3:20 Paper 214a: Modeling Continuous Enzymatic Reactive Crystallization of β-Lactam Antibiotics — ***Matthew A. McDonald****, Andreas S. Bommarius, Martha A. Grover, Ronald W. Rousseau*

3:40 Paper 214b: Continuous Crystallization-Milling Processes: Guaranteeing the Manufacture of Stable Polymorphs — *Till Köllges,* ***Thomas Vetter***

4:00 Paper 214c: Micro-Scale Process Development and Optimization for Crystallization Processes — ***Niall Mitchell****, Cameron Brown, Sean Bermingham*

4:20 Paper 214d: Continuous Crystallization Process for Resolution of Diastereomeric Salts: Ibuprofen Lysine Case Study — ***Melba Simon****, Roderick Jones, Philip Donnellan, Brian Glennon, Steven Ferguson*

4:40 Paper 214e: Ultrasound-Assisted Crystallization in a Two-Stage Continuous MSMPR Crystallizer System — *Zhenguo Gao, Dan Zhu, Yuanyi Wu,* ***Sohrab Rohani****, Junbo Gong, Jingkang Wang*

5:00 Paper 214f: Membrane-Assisted Antisolvent Crystallization for the Continuous and Accurate Control of Pharmaceuticals Manufacture — ***Xiaobin Jiang, Linghan Tuo****, Gaohong He*

5:20 Paper 214g: Rapid Crystallization Development Through Automation of Solubility Screening Coupled with XRPD — ***Christopher J. Morrison****, Christopher Nunn, Yan Sun*

5:40 Concluding Remarks

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(215) Development of Sustainable New Materials and Intermediates
Monday, Oct 30, 3:15 PM
MCC, 102B

Tom Xu, Chair
Shaibal Roy, Co-Chair

Sponsored by:
Process Research and Innovation

3:15 Paper 215a: Production of Chemicals from the Thermal Cracking of Castor Oil, Castor Oil Methyl Ester and Ricinoleic Acid — *Vanderlei R. da Costa, Vinicyus R. Wiggers, Vanderleia Botton, Edésio L. Simionatto, Dilamara R. Sharf, Henry F. Meier,* ***Laércio Ender***

3:37 Paper 215b: Neem-Coated Urea: A Fiscal Approach for Farmers — ***Sara Ahsan****, Ali Ayub*

3:59 Paper 215c: Technoeconomic Assessment of Two-Step Process for Upgrading and Utilizing Used Railroad Ties in an Integrated Biorefinery — ***Nourredine Aboulmoumine****, Ross Houston*

4:21 Paper 215d: Valorisation of Three-Phase Olive Mill Wastewater with the Addition of High-Protein Co-Substrates — *Dimosthenis Sarigiannis, Stavros Zachariou, Marilena Lioti, Fokion Kaldis,* ***Ioannis Zarkadas***

4:43 Paper 215e: Evaluation and Comparison of the Scale-Up Potential for Autotropic and Heterotrophic Algal Oil Production — ***Jasmine Kreft****, Wayne S. Seames, Nickolas Garcia, Eric Moe*

5:05 Paper 215f: Process Developments in Continuous Silicone-Polyether Copolymers — ***Akshay Kundan****, Chauncey Rinard, Steven Bahr*

5:27 Paper 215g: Esterification of Carboxylic Acids Present in the Bio-Oil Produced by Thermal Cracking of Triacylglycerols — *Eloá S. Ramos, Laércio Ender, Vanderleia Botton, Dilamara R. Sharf, Edésio L. Simionatto, Henry F. Meier,* ***Vinicyus R. Wiggers***

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(216) Electrocatalysis and Photoelectrocatalysis III: Computational Methods
Monday, Oct 30, 3:15 PM
MCC, L100D

Unmesh Menon, Chair
Jason Goodpaster, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

3:15 Paper 216a: Generalizing the Design Principles of Pt-Based Alloy Catalysts with Improved ORR Performance and Durability — ***Zhenhua Zeng****, Jeffrey P. Greeley*

3:33 Paper 216b: Computational Insights into Thermal and Photoresponse of Pd/C and Pd/N Co-Doped TiO_2 Using DFT — ***Sai Phani Kumar Vangala****, Parag Arvind Deshpande*

3:51 Paper 216c: Transition Metal-Doped C_2N as Active Catalysts for the Oxygen Reduction Reaction — *Anjli M. Patel,* ***Ambarish R. Kulkarni****, Jens K. Nørskov*

4:09 Paper 216d: Electrochemical Synthesis of Hydrogen Peroxide via Water Electrolysis: Challenges and Opportunities — ***Samira Siahrostami****, Jens Nørskov*

4:27 Paper 216e: Modeling Electrochemical Reactions: DFT-Based Models Including Explicit Solvation, Electrolyte, and Electrochemical Potential — ***Jason Goodpaster***

4:45 Paper 216f: Efficiently Determining Solvent Effects at Metal-Water Interfaces — *Satish Iyemperumal,* ***N. Aaron Deskins***

5:03 Break

5:21 Paper 216h: Machine-Learning Model Development for Electrocatalyst Discovery — ***Zheng Li****, Hongliang Xin*

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(217) Energy & the Environment U.G. Research Session (Invited Talks)
Monday, Oct 30, 3:15 PM
MCC, 101H

Srihari K. Maganti, Chair
Tianxing Cai, Co-Chair

Sponsored by:
Young Professionals Committee (YPC)

3:15 Paper 217b: Flex-to-Stretch Electronics — ***Steven Erlenbach***

3:40 Paper 217c: Systematic Analysis of Cloud Point and Crystallization in Fatty Acid Ethyl Ester Biodiesel Mixtures — ***Patrick Leggieri***

4:05 Paper 217d: Feasibility Study of Ionic Liquid Desalination Design — ***Zachary Cosenza***

4:30 Paper 217a: Preparation and Characterization of Shape Memory Assisted Self-Healing Coatings — ***Evelyn Korbich***

4:55 Paper 217e: Defluoridation of Ground Water Using Impregnated Aluminum — ***Muhammad Awais Jamali***

5:20 Paper 217f: Ordering pH-Responsive Polymer-Grafted Nanoparticles in Flow Coating Process — ***T. Carlson***

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(218) Faculty Candidates in CoMSEF II: Energy, Catalysis, and Interfaces
Monday, Oct 30, 3:15 PM
MCC, L100H

M. Scott Shell, Chair
Amir Haji-Akbari, Co-Chair

Sponsored by:
Computational Molecular Science and Engineering Forum

3:15 Paper 218a: Rational Design of Alloyed Materials for Energy Conversion — ***Liang Zhang***

3:30 Paper 218b: Climbing the Volcano: Active-Site Engineering at the Atomic Scale — ***Joseph H. Montoya***

3:45 Paper 218c: Developing Ab-Initio Methodology for Advancing Catalytic Reactions — ***Eric Walker***

4:00 Paper 218d: First-Principles-Derived Structure-Energy Relationship for Surface Oxides — ***Alexander V. Mironenko****, Dionisios G. Vlachos*

4:15 Paper 218e: First-Principles-Based Design of Reaction Conditions for the Catalytic Conversion of Methane to Methanol over Cu-Exchanged SSZ-13 — ***Florian Göltl****, Manos Mavrikakis*

4:30 Paper 218f: Reaction Ensemble Monte Carlo Simulations of Xylene Isomerization Under Confinement — ***Ryan Gotchy Mullen****, Edward J. Maginn*

4:45 Paper 218g: Understanding Separation and Catalysis in Nanoporous Materials — ***Peng Bai***

5:00 Paper 218h: Modeling Self-Assembly of Metal-Organic Frameworks with Enhanced Sampling Techniques — ***Yamil J. Colón****, Ashley Guo, Lucas Antony, Kyle Hoffmann, Juan de Pablo*

5:15 Paper 218i: Computationally Efficient High-Throughput Screening of Metal-Organic Frameworks for Hydrogen Storage — ***N. Scott Bobbitt****, Arun Gopalan, Benjamin Bucior, Jiayi Chen, Randall Q. Snurr*

5:30 Paper 218j: Effects of Ion Self-Energy on the Double-Layer Structure and Properties at the Dielectric Interface — ***Rui Wang***

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(219) Free Forum on Engineering Education: Junior and Senior Years II
Monday, Oct 30, 3:15 PM
MCC, 205C

Jennifer Cole, Co-Chair
Christy Wheeler West, Co-Chair

Sponsored by:
Undergraduate Education

3:15 Paper 219a: Industrial Safety Curriculum for Chemical Engineering Education — ***Juanita Miller****, David Rockstraw*

3:33 Paper 219b: Using AIChE's Concept Warehouse to Help Teach Process Safety–Related Engineering Science — ***Bruce K. Vaughen***

3:51 Paper 219c: Process Safety Education Using Simulators in a Chemical Engineering Operations Center Experience — ***Robert G. Bozic****, Matthew B. Garvey, Donald C. Glaser*

4:09 Paper 219d: Training Our Upcoming Chemical Engineers by Simulating an Industrial Setting: A Classroom Case Study on Waste Cellulose Valorization — ***Anton De Vylder****, Alexandra Bouriakova, Kenneth Toch, Joris W. Thybaut*

4:27 Paper 219e: Design Simulation for the Process Industries: An Inter-Institutional Initiative for Chemical Engineering Education in Ireland — ***Federico Orefice****, Darragh Coakley, Philip Donnellan, David Dorran, Noel Duffy, Brian Freeland, Carmel Hensey, Witold Kwapinski, Damian Mooney, Gearoid O. Suilleabhain, Jorge Oliveira, Michael O'Mahony, Brian Glennon, Joe Hannon, John Milne, Kevin Smyth, Patricia Kieran*

4:45 Paper 219f: Tutorial: SMART-CN Education Modules for Senior Undergraduate or Graduate Engineering Curriculum — ***Debalina Sengupta****, Yinlun Huang, Thomas F. Edgar, Cliff Davidson, Mario Richard Eden, Mahmoud El-Halwagi*

5:03 Paper 219g: Dual Learning in (Chemical) Engineering: From Theory to Practice — *Laureano Jiménez Esteller, Dieter Thomas Boer,* ***Carlos Pozo Fernández***

5:21 Paper 219h: A Graduate Course in Research Data Management — ***Joseph Holles****, Lawrence Schmidt*

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(220) Fuel Cell Membranes
Monday, Oct 30, 3:15 PM
MCC, M100I

W. S. Winston Ho, Co-Chair
Peter N. Pintauro, Co-Chair
He Bai, Co-Chair

Sponsored by:
Membrane-Based Separations

3:15 Paper 220a: Performance Evaluation of a Hybrid Hydrogen-Vanadium Reversible Fuel Cell — ***Trung V. Nguyen****, Regis Dowd Jr., Vikram Lakhanpal, Devon Powers, Ryszard Wycisk, Peter N. Pintauro*

3:33 Paper 220b: Fuel Cell Membranes with Enhanced Durability and Performance Based on Fluoroelastomers Functionalized with Heteropoly Acids — ***Andrew M. Herring****, Andrew R. Motz, Tara P. Pandey, Mei-Chen Kuo*

3:51 Paper 220c: Hydroxylated Graphane: An Anhydrous Proton Exchange Membrane — ***Abhishek Bagusetty****, Pabitra Choudhury, J. Karl Johnson*

4:09 Paper 220d: Interfacial Transport Resistances and Coupled Transport — ***Jay Benziger****, Ioannis G. Kevrekidis, Michal Pavelka, Vaclav Klika*

4:27 Paper 220e: Exploring Ionomer-Related Transport Phenomena in Polymer-Electrolyte Fuel Cells — ***Adam Weber***

4:45 Paper 220f: Structured Ion-Exchange Membrane-Electrode Interfaces Fabricated via Conventional and Advanced Block Copolymer Lithography — *Le Zhang,* ***Christopher G. Arges***

5:03 Paper 220g: Highly Durable Aromatic Anion-Exchange Membranes for Solid Alkaline Fuel Cells — ***Takeo Yamaguchi****, Shoji Miyanishi, Hidenori Kuroki*

5:21 Paper 220h: Sustainion™ Membranes for Carbon Dioxide and Alkaline Water Electrolyzers — ***Claire Hartmann-Thompson****, John Baetzold, Mark Pellerite, Syed Dawar Sajjad, Jerry Kaczur, Yan Gao, Zengcai Liu, Marina Kaplun, Hongzhou Yang, Richard I. Masel, Steve Solomonson, Laura Nereng, Dale Lutz*

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(221) Fuel Cells, Electrolyzers, and Electrochemical Devices
Monday, Oct 30, 3:15 PM
MCC, 200F

Yangchuan Xing, Chair

Sponsored by:
Transport and Energy Processes

3:15 Paper 221b: Session Keynote: Economics of Large-Scale Hydrogen Generation: Can H_2 Compete with Batteries? — ***Cortney Mittelsteadt***

3:34 Paper 221c: Session Keynote: Utilizing Proton Exchange Membrane (PEM) Electrolyzers as a Robust Platform for Emerging Electrochemical Technologies — ***Julie N. Renner****, Wayne Gellett, Lauren F. Greenlee, Shelley D. Minteer, Katherine Ayers*

3:53 Paper 221d: Demonstration of Hydrogen Production by Multi-Typed Solid Oxide Electrolysis Cells System — ***Naomi Tsuchiya****, Hisao Ohmura, Shohei Kanamura, Masato Yoshino, Seiji Fujiwara, Tsuneji Kameda, Masahiko Yamada, Kazuya Yamada*

4:12 Paper 221e: A High-Performing Alkaline Water Electrolyzer — *Zengcai Liu, Yan Gao, Hongzhou Yang, Syed Dawar Sajjad, Jerry Kaczur,* ***Richard I. Masel***

4:31 Paper 221f: Iridium Nanowires as Highly Active, Oxygen Evolution Reaction Electrocatalysts — ***Shaun M. Alia****, Sarah Shulda, Chilan Ngo, Svitlana Pylypenko, Bryan S. Pivovar*

4:50 Paper 221g: The Effect of Two Different Preparation Methods of Cu@Pd/C in Direct Formic Acid Fuel Cell — ***Bita Khorasani****, Louis Scudiero, Su Ha*

5:09 Paper 221h: Enhanced Performance with Ni-Based Single Solid Oxide Fuel Cells with Mo-CZ Composition — ***Xiaoxue Hou****, Kai Zhao, Grant Norton, Su Ha*

5:28 Paper 221i: Invited Talk — ***Whitney G. Colella***

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(222) Fuels from the Sun: Nanomaterials for Water Splitting, Artificial Photosynthesis, and Other Photocatalytic and Photoelectrochemical Reactions
Monday, Oct 30, 3:15 PM
MCC, 200G

James G. Radich, Chair
Adam Holewinski, Co-Chair

Sponsored by:
Nanomaterials for Applications in Energy and Biology

3:15 Paper 222a: Fabrication of Homologous TiO_2/NH_2-MIL-125(Ti) Heterojunction for Efficient Visible-Light-Induced Aerobic Oxidation of Benzyl Alcohol and Degradation of Tetracycline — ***Xiyi Li****, Yunhong Pi,* ***Zhong Li****,* ***Jing Xiao***

3:37 Paper 222b: Mid-Infrared Surface Plasmon-Enhanced Molecular Desorption — ***Weize Hu****, Michael A. Filler*

3:59 Paper 222c: SiO_2 as a Protective Layer in Visible-Light-Induced Hydrogen Production — ***Rong Zhao****, James G. Radich*

4:21 Paper 222d: Plasmonic Purification: Visible-Light-Driven Generation of Reactive Oxygen Species for Water Disinfection — ***Daniel Willis****, Sara K. F. Stofela, Katrina Taylor, Kevin M. McPeak*

4:43 Paper 222e: Efficient Photoreduction of Bicarbonate to Formate Catalyzed by Gold-TiO_2 Composite Nanocatalyst Under Solar Light — *Hanqing Pan, Alexzander Steiniger, Michael D. Heagy,* ***Sanchari Chowdhury***

5:05 Paper 222f: Solution Combustion Synthesis and Photoelectrochemistry of $Ga_xZn_{1-X}O_yN_{1-Y}$ — ***Ben Meekins***

5:27 Paper 222g: Mixed Oxide–Based Redox Catalysts for Hydrogen and Liquid Fuel Co-Generation via a Hybrid Solar-Redox Scheme — ***Vasudev Pralhad Haribal****, Feng He, Amit Mishra, Fanxing Li*

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(223) Fundamentals of Fluidization III: Experimental Findings
Monday, Oct 30, 3:15 PM
MCC, 200I

Sarah E. Mena, Co-Chair
Manuk Colakyan, Co-Chair

Sponsored by:
Fluidization and Fluid-Particle Systems

3:15 Paper 223a: Investigating Cylindrical Particle Fluidization Using X-Ray Particle Tracking Velocimetry (XPTV) — *Xi Chen, Wenqi Zhong,* ***Theodore J. Heindel***

3:32 Paper 223b: Assessing Agglomerate Characteristics in a Nanopowder Fluidized Bed
— ***J. Ruud van Ommen***, *Andre Fabre, Samir Salameh, Michiel T. Kreutzer*

3:49 Paper 223c: Solids Mixing in Fluidized-Bed Systems Using Fluorescence Tracer Method
— ***Shyam Sundaram***, *S. B. Reddy Karri, Ray Cocco*

4:06 Paper 223d: Conditions for Pattern Formation in Pulsed Fluidized Beds — ***Kaiqiao Wu***, *Victor Francia, Marc-Olivier Coppens*

4:43 Paper 223e: Evaluation of Spouted Bed Flow Instabilities via High-Speed Video and Pressure Fluctuations
— ***Steven Rowan***, *Jingsi Yang, Ronald W. Breault, Justin Weber*

4:57 Paper 223g: Electrical Capacitance Volume Tomography Studies of Characteristics of Gas-Solid Slugging Fluidization with Geldart Group D Particles Under Elevated Temperatures — ***Dawei Wang***, *Mingyuan Xu, Yaswanth Pottimurthy, Andrew Tong, Qussai Marashdeh, Benjamin Straiton, Pengfei He, Liang-Shih Fan*

5:14 Paper 223h: Local Agglomeration Measurements of Mildly Cohesive Particles in a Dilute Riser
— ***Casey Q. LaMarche***, *Haley Manchester, Peiyuan Liu, Kevin M. Kellogg, Christine M. Hrenya*

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(224) Fundamentals of Food, Energy, and Water Systems
Monday, Oct 30, 3:15 PM
MCC, 102A

Heriberto Cabezas, Chair
JoAnn S. Lighty, Co-Chair

Sponsored by: Fundamentals

3:15 Paper 224a: Evaluating Combined Heat and Power Deionization Systems for Efficient Water Reuse at Thermoelectric Power Plants
— ***Marta Hatzell***, *Jiankai Zhang*

3:40 Paper 224b: Biochar Amendments for Increased Crop Yields: How Can Biochars Improve Crop Nutrient Availability?
— *Yi Chen*, ***Kyriacos Zygourakis***

4:05 Paper 224c: Moisture Retention in Emulated Soil Micromodels: Development and Performance of Sustainable Agriculture Biotechnology
— ***Yi-Syuan Guo***, *Brian C. Cruz, Daniel P. Dougherty, Jessica F. Chau, Leslie M. Shor*

4:30 Paper 224d: Molecular Modeling and Simulation Studies of the Structural and Energetic Evolution During Dehydration of Food Systems
— ***Jee-Ching Wang***, *Athanasios I. Liapis*

4:55 Paper 224e: Metallic Membranes for N_2 Separation and NH_3 Production
— ***Simona Liguori***, *Kyoungjin Lee, Jennifer Wilcox*

5:20 Paper 224f: Capacitive Deionization of Brackish Water for Irrigation and Energy Storage
— ***Vander Wal Randy***, *Ramakrishan Rajagopalan, Arupananda Sengupta*

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(225) High-Pressure Phase Equilibria and Modeling
Monday, Oct 30, 3:15 PM
MCC, M100C

Christopher L. Kitchens, Chair

Sponsored by: High Pressure

3:15 Paper 225a: Discovery of the Universal Van Der Waals Generic Cubic Equation of State for the Continuity of Gaseous and Liquid States of Fluids and Mixtures — ***Akanni S. Lawal***

3:35 Paper 225b: Vapor-Liquid Equilibrium Data for the Systems H_2S-MDEA-H_2O and CH_4-H_2S-MDEA-H_2O at High Solvent Concentrations and High Pressures — ***Eirini Skylogianni***, *Diego D. D. Pinto, Hanna K. Knuutila, Christophe Coquelet*

3:55 Paper 225c: Solubility of Timolol Maleate in Supercritical Carbon Dioxide with Water on Extraction from Silicone Hydrogel — ***Yusuke Shimoyama***, *Yuta Yokozaki*

4:15 Paper 225d: Experimental and Modelling Study of the Phase Behaviour of (CO_2 + CH_4 + Methylbenzene) at High-Pressure and High-Temperature Conditions
— *Saif Al Ghafri*, ***J. P. Martin Trusler***

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(226) In-Situ and Operando Spectroscopy of Catalysts
Monday, Oct 30, 3:15 PM
MCC, L100F

Nicholas Brunelli, Chair
Juan J. Bravo-Suarez, Co-Chair
George Tsilomelekis, Co-Chair
Joshua Gorimbo, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

3:15 Paper 226a: Revealing Catalytic Active Units of Ru for NH_3 Decomposition by *Operando* XPS
— ***Weiqing Zheng***, *Jian Zhang, Dangsheng Su, Robert Schloegl*

3:35 Paper 226b: Quantitative and Atomic-Scale View of CO-Induced Pt Nanoparticle Surface Reconstruction at Saturation Coverage and Implications for CO Oxidation Structure Sensitivity
— ***Matthew Kale***, *Talin Avanesian, Sheng Dai, George W. Graham, Xiaoqing Pan, Phillip Christopher*

3:55 Paper 226c: *Operando* Electrochemical Grazing Incidence X-Ray Absorption and Diffraction for CO_2 Reduction on AuPd, Pd and Au Electrodes — ***Jeremy T. Feaster***, *Maryam Farmand, John Lin, Alan Landers, Sean Fackler, Drew Higgins, Yusaku F. Nishimura, Ryan Davis, Apurva Mehta, Junko Yano, Thomas F. Jaramillo, Walter Drisdell*

4:15 Paper 226d: Chemical Transient Kinetics in Studies of the CO Hydrogenation Mechanism over Co-Based Catalysts
— ***Motahare Athariboroujeny***, *Viacheslav Iablokov, Greg Collinge, Norbert Kruse, Jean-Sabin McEwen*

4:35 Paper 226e: In-Situ FTIR Studies of Ethanol Conversion on Zr-KIT-5 and Zr-KIT-6 Catalysts — ***Priya Srinivasan***, *Maria Ramirez, Juan J. Bravo-Suarez*

4:55 Paper 226f: Mechanistic and Spectroscopic Evidence for Reactive Intermediate Structures During C-O Bond Rupture in Small Oxygenates on Metal Phosphide Clusters
— ***Megan E. Witzke***, *Abdulrahman Almithn, Christian L. Coonrod, Mark D. Triezenberg, David D. Hibbitts, David W. Flaherty*

5:15 Paper 226g: Insight into the Structure Evolution of Iron-Based Catalysts for Hydrogenation of CO/CO_2 Using *Operando* Techniques
— *Yulong Zhang, Yang Sun, Zhengpai Zhang, Pengfei Tian, Jing Xu, Huiping Li*, ***Yifan Han***

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(227) In Honor of Bill Koros II
Monday, Oct 30, 3:15 PM
MCC, M100H

Ryan Lively, Chair
Ingo Pinnau, Co-Chair
Ali A. Rownaghi, Co-Chair

Sponsored by:
Membrane-Based Separations

3:15 Paper 227a: Membrane Materials for Gas Separations
— ***Benny D. Freeman***

3:37 Paper 227b: Molecular Sieve Nanosheets for Membrane Applications
— ***Michael Tsapatsis***

4:02 Paper 227c: Carbon Molecular Sieve Membranes for Applications in Olefins Units — ***Liren Xu***, *Mark Brayden, Marcos Martinez*

4:24 Paper 227d: High-Flux Thermally Rearranged (TR) Hollow Fiber Membranes for Gas Separation
— ***Young Moo Lee***

4:46 Paper 227e: Polymeric Membranes for High-Temperature Gas Separations — ***Mary E. Rezac***

5:08 Paper 227f: Mixed-Matrix Membranes for Organic Solvent Nanofiltration — ***Andrew Livingston***

5:30 Paper 227g: Membranes for CO_2 Capture: A Green Technology for Large and Small Industrial Applications
— ***May-Britt Hagg***

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(228) In Honor of Stuart W. Churchill II (Invited Talks)
Monday, Oct 30, 3:15 PM
MCC, 101E

Warren D. Seider, Chair
Peter Lederman, Co-Chair

Sponsored by:
Transport and Energy Processes

3:15 Paper 228a: Teaching the Need to Account for Mixing in the Design of Tubular Reactors as Recommended by Stuart Churchill — ***Warren D. Seider***

3:45 Paper 228b: Clustering of Heavy Particles in Turbulence: Dimensional Analysis and Scaling Laws in the Inertial Range — ***Lance R. Collins***

4:15 Paper 228c: Measurements and Prediction of Sooting Tendencies of Hydrocarbons and Oxygenated Hydrocarbons — ***Drubajyoti Das***, *Peter St. John, Charles S. McEnally, Seonah Kim, Lisa D. Pfefferle*

4:45 Paper 228d: Role of Brain Interstitial Transport in Alzheimer's Disease — ***Christina Chan***, *Neil Wright, Bingmei Fu*

5:15 Paper 228e: Farewell
— ***Warren D. Seider***

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(229) Medical Devices
Monday, Oct 30, 3:15 PM
MCC, 202A/B

Bernard Van Wie, Chair
Erica Ricker, Co-Chair

Sponsored by:
Chemical Engineers in Medicine

3:15 Paper 229a: Combined Treatment of Heat and Antibiotics to Mitigate Biofilms on Implanted Devices
— ***Erica Ricker***, *Eric Nuxoll*

3:36 Paper 229b: Rapid Separation of Bacteria from Whole Blood for Sepsis Diagnosis — ***Mahsa Alizadeh***, *William G. Pitt, Daniel Mc Clellan, Colin Bledsoe, Rae Blanco, Alex Hunter, Caroline Hickey, Madison Wood, Alexandra Carter, Evelyn Welling*

3:57 Paper 229c: Characterization of TiO_2 Nanotubular Sensor for Detecting Tuberculosis Volatile Organic Compounds — ***Yalda Saffary***, *Christina Willis, Manoranjan Misra, Swomitra Mohanty*

4:18 Paper 229d: Novel Reverse-Electrodialysis Biofuel Cell
— ***Christa N. Hestekin***, *Jamie Hestekin, Brigitte Rodgers, Chase Smith*

4:39 Paper 229e: Nanocomposite for Implantable Electronic Devices
— ***Frank Curry Jr.***, *Huanan Zhang*

5:00 Paper 229f: Wireless, Battery-Free Optofluidic Device for Programmable Fluid Delivery and Optogenetics — ***Yi Zhang***, *Philipp Gutruf, Daniel Castro, Michael R. Bruchas, John A. Rogers*

5:21 Paper 229g: Biomimicry in a High–Cell Population Density Perfusion Centrifugal Bioreactor
— ***Bernard J. Van Wie***, *Nehal I. Abu-Lail, Arda Gozen, William Davis, Juana Mendenhall, Mahmoud Amr, Alia Mallah, Arshan Nazempour, Chrystal Quisenberry, Christopher Detzel, Baran Arslan, David Kidwell, Gaber Abdellrazeq, Mahmoud Elnaggar*

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(230) Mixing in Rheologically Complex Fluids
Monday, Oct 30, 3:15 PM
MCC, 102D

François Bertrand, Chair
Li Xi, Co-Chair

Sponsored by:
North American Mixing Forum

3:15 Paper 230a: Industrial-Scale Modeling of Herschel-Bulkley (Yield Stress) Fluids
— ***John A. Thomas***, *Kevin Smith*

3:40 Paper 230b: Viscometer for On-Site Rheology Measurements: Development and Application
— ***Richard K. Grenville***, *Jason J. Giacomelli, Wojciech Wyczalkowski, Addison Root*

4:05 Paper 230c: Using μ^2rheology to Measure Rheological Properties During Repeated Phase Transitions of Hydrogenated Castor Oil
— ***Matthew Wehrman***, *Seth Lindberg, Kelly M. Schultz*

4:30 Paper 230d: Model Systems for Mixed Particulate Fermentation Broth
— *Matthias Kraume*, ***Lutz Böhm***, *Chrysoula Bliatsiou*

4:55 Paper 230e: Polycarboxylate Ether Cement Superplasticizers Containing Copolymer Backbones with Improved Rheology Performance — ***Xue Chen***, *Jennifer Lowe, Thomas Clark, Mike Radler*

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(231) Multiphase Reaction Engineering
Monday, Oct 30, 3:15 PM
MCC, L100A

Vaibhav Kelkar, Chair
Xinrui Yu, Co-Chair
Sagar Sarsani, Co-Chair
Alan Stottlemyer, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

3:15 Paper 231a: Results of Packed-Bed Reactor Experiment on the International Space Station
— ***Brian J. Motil***, *Vemuri Balakotaiah, Enrique Rame, Paul Salgi*

3:37 Paper 231b: Avoiding Fluidization in 3-Phase Packed-Bed Reactors
— ***Justin Walker***, *Suraj Deshpande, Daniel A. Hickman*

3:59 Paper 231c: Residence Time Distribution Studies in a Laboratory-Scale Trickle-Bed Reactor for Liquid-Phase Hydrogenation of Acetylene — ***Humayun Shariff***, *Premkumar Kamalanathan, Muthanna Al-Dahhan*

4:21 Paper 231d: Numerical Simulation of the Bubble Column with a CFD-PBM Coupled Model: Importance of the Drag Force of Bubble Swarms
— ***Tiefeng Wang***, *Guangyao Yang*

4:43 Paper 231e: Low-Order Modeling of the Vapor-Phase Upgrading of Fast-Pyrolysis Bio-Oil in a Bubbling Fluidized-Bed Reactor
— ***Jonathan E. Sutton***, *Gavin Wiggins, C. Stuart Daw*

5:05 Paper 231f: A Sustainable Waste Management Alternative: Catalytic Gasification — *Eric M. Lange*, ***Uchechukwu Obiako***, *Samuel Sanya, Stephen A. Reeves, Aliandra D. Barbutti, Jorge E. Gatica*

5:27 Paper 231g: Design and Optimization of Multiphase FCC Regenerator Hydrodynamics Coupled with Reaction Kinetics — ***Sagar Srinivas***

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(232) Novel Approaches to CO_2 Utilization
Monday, Oct 30, 3:15 PM
MCC, 200C

Lynn Brickett, Chair
Rameshwar Srivastava, Co-Chair

Sponsored by:
Advances in Fossil Energy R&D

3:15 Paper 232a: High-Performance CO_2 Electrolyzers — ***Richard I. Masel***, *Zengcai Liu, Hongzhou Yang, Yan Gao, Syed Dawar Sajjad, Jerry Kaczur, Claire Hartmann-Thompson, Marina Kaplun, Mark Pellerite, John Baetzold, Krzysztof Lewinski, Laura Nereng, Dale Lutz, Steve Solomonson*

3:37 Paper 232b: CO Conversion to Selected Chemicals Using Electrochemically Generated CO from CO_2 — ***Jerry Kaczur***, *Zengcai Liu, Hongzhou Yang, Richard I. Masel*

4:43 Paper 232c: Nano-Engineered Catalyst for the Utilization of CO_2 in Dry Reforming to Produce Syngas
— ***Shiguang Li***, *Zeyu Shang, Xinhua Liang*

4:21 Paper 232d: Ethylene Production from Shale- and Coal-Derived Flue Gases — ***Jadid Samad***, *Amit Goyal*

4:31 Paper 232e: CO_2 Utilization in the Production of Ethylene Oxide
— ***Paul Mobley***, *Jonathan Peters, Nandita Akunuri, Marty Lail*

5:05 Paper 232g: Pulse/Pulse-Reverse Electrodeposition of Gas-Diffusion Electrocatalysts for CO_2 Reduction
— ***Brian T. Skinn***, *Sujat Sen, Timothy D. Hall, Maria Inman, E. Jennings Taylor, Fikile Brushett*

5:27 Paper 232h: Process Intensification for Electrochemical Utilization of CO_2 — ***Leland R. Widger***, *Jesse G. Thompson, Kunlei Liu*

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(233) Population Balance Modeling for Particle Formation Processes: Nucleation, Aggregation, and Breakage Kernels
Monday, Oct 30, 3:15 PM
MCC, 200H

Dana Barrasso, Chair
R. Bertrum Diemer Jr., Co-Chair

Sponsored by:
Particle Production and Characterization

3:15 Paper 233a: Population Balance Modeling of Breakage of High–Aspect Ratio Crystals in Stirred Slurries
— ***Priscilla Hill***

3:33 Paper 233b: Population Balance Equation for Calculation of the Inlet Distribution for Oil and Water Droplets in Continuous Gravity Separators — ***Christoph Josef Backi***, *Brian Arthur Grimes, Sigurd Skogestad*

3:51 Paper 233c: Data-Driven Model for the Prediction of Particle Size Distribution from Measured Chord-Length Distribution: Model Extensions and Application to Population Balance Model Identification
— ***Roberto Irizarry***, *Jochen Schoell, Lorenzo Codan*

4:09 Paper 233d: Population Balance: The Auto-Catalytic Nature of Secondary Nucleation in Seeded Batch Crystallizations — ***Rory Tyrrell***, *Brian de Souza, P. J. Frawley*

4:27 Paper 233e: DEM-Based Prediction of Critical Impact Velocities of Aggregation and Breakage and Daughter Distributions of Cohesive Powders — ***Kevin M. Kellogg***, *Peiyuan Liu, Casey Q. LaMarche, Christine M. Hrenya*

4:45 Paper 233f: Towards a General Model for Twin-Screw Wet Granulation: Development and Calibration of a Novel Three-Compartmental PBM Model — ***Daan Van Hauwermeiren***, *Maxim Verstraeten, Kai Lee, Neil Turnbull, Pankaj Doshi, Mary T. am Ende, Thomas De Beer, Ingmar Nopens*

4:59 Paper 233g: Towards a General Model for Twin-Screw Wet Granulation: Validation of a PBM Model Through Linking Calibrated Model Parameters to Process Conditions
— ***Daan Van Hauwermeiren***, *Maxim Verstraeten, Kai Lee, Pankaj Doshi, Mary T. am Ende, Thomas De Beer, Ingmar Nopens*

5:13 Paper 233h: Towards a General Model for Twin-Screw Wet Granulation: Application of a Novel Validated PBM Model to a Hydrophilic Compound and Linking Model Parameters to Blend Properties
— ***Daan Van Hauwermeiren***, *Maxim Verstraeten, Kai Lee, Neil Turnbull, Mary T. am Ende, Thomas De Beer, Ingmar Nopens*

5:27 Paper 233i: Population Balance Modeling Applied to the Milling of Hot-Melt Extrudates — ***Maxx Capece***, *John C. Strong, Oliver Heinzerling, Ping Gao*

(234) Poster Session: Fluid Mechanics
Monday, Oct 30, 3:15 PM
Hilton, Marquette I/II/III/VIII/IX

Sibani Lisa Biswal, Chair
John M. Frostad, Co-Chair

Sponsored by: Fluid Mechanics

■ COLLOIDAL HYDRODYNAMICS: STRUCTURE AND MICRORHEOLOGY

Paper 234a: Microscale Acoustic Streaming Flows in Viscoelastic Fluids: Comparison of Experiment and Simulation — ***Behrouz Behdani***, *Ran Zhou, Cheng Wang, Joontaek Park*

Paper 234c: Influence of Cell Lengths on Surface Drag in Motile Bacteria — ***Katie Ford***, *Pushkar Lele*

Paper 234d: Dynamics of Semiflexible Colloidal Particle Chains Under Rotating Magnetic Fields — ***Steve Kuei***, *Sibani Lisa Biswal*

Paper 234e: A Study of the Dynamics of Human Pedestrians Using Experiments and Simulations in the Indian Context — ***Indranil Saha Dalal***, *Anurag Tripathi, Amullya Kale, Ishan Prashant*

■ COMPLEX FLUIDS: MACROMOLECULES AND SELF-ASSEMBLY

Paper 234f: Extensional Rheometry with a Handheld Mobile Device — *Kristin A. Marshall, Aleesha M. Liedtke, Anika H. Todt,* ***Travis W. Walker***

Paper 234g: Free Surface Flows and Extensional Rheology of Polymer Solutions — ***Jelena Dinic***, *Leidy N. Jimenez, Vivek Sharma*

Paper 234h: Rheological Behavior of Poly(vinyl alcohol) in Aqueous Solutions: Comparison and Assessment of Rheological Parameters Obtained by Empirical Correlations — ***Maria Veronica Carranza Oropeza***, ***Luis Carrasco Venegas Sr.***, *Sandy Candiotti Velasquez*

■ HYDRODYNAMICS OF BIOLOGICAL SYSTEMS

Paper 234i: The Phantom Generation of a Complex Nasal Geometry with Horizontal Cut for LDA Measurements — ***Manuel Berger***, *Martin Pillei, Andreas Mehrle, Wolfgang Recheis, Florian Kral, Wolfgang Freysinger, Michael Kraxner*

Paper 234j: Using LAOS and Transient Data to "Fingerprint" Human Blood Rheological Data — ***Tyler Helton***, *Matthew Armstrong*

Paper 234k: Using Rheology to Improve Blood-Flow Models — ***Jeffrey S. Horner***

Paper 234l: Comparison of Simple Rheological Models in Fitting and Predicting Steady-State and Transient Blood Rheology — ***Michael Deegan***, ***Evan Ousley***, *Matthew Armstrong*

Paper 234m: Blood Rheology — ***Jeffrey S. Horner***

■ INTERFACIAL & NONLINEAR FLOWS MICROFLUIDIC AND MICROSCALE FLOWS

Paper 234o: Development of Predictive Model for Sizes of Gas and Liquid Slugs Formed in Millimeter-Scale T-Shaped Channels — ***Gwangnoh Ahn***, *Osamu Tonomura, Satoshi Taniguchi, Aoyama Tomoya, Shinji Hasebe*

■ PARTICULATE AND MULTIPHASE FLOWS: COLLOIDAL AND GRANULAR SYSTEMS

■ PARTICULATE AND MULTIPHASE FLOWS: DYNAMICS OF EMULSIONS, BUBBLES, DROPLETS

Paper 234p: Shape Evolution and Spreading of Liquid Droplets in Miscible Environments — ***Dan Walls***, *Simon Haward, Amy Shen, Gerald G. Fuller*

Paper 234q: Impact Forces of Inertia-Driven Liquid Drops — ***Ting-Pi Sun***, *Leonardo Gordillo, Xiang Cheng*

Paper 234r: Visualizing Nanoscopic Topography, Patterns, Flows, Thickness Transitions and Instabilities in Stratifying Freestanding Thin Films — *Yiran Zhang, Subinuer Yilixiati,* ***Vivek Sharma***

Paper 234s: Contrasting Drainage and Stratification in Horizontal vs. Vertical Micellar Foam Films — ***Subinuer Yilixiati***, *Ewelina Wojcik, Yiran Zhang, Vivek Sharma*

Paper 234t: Solvent Effects on the Crystallinity of Petroleum Asphaltenes — ***Yuan Yang***, *Thomas Headen, Michael P. Hoepfner*

Paper 234u: The Impact of Slurry Concentrations on Bubble Properties in Pilot-Scale Bubble Column with Industrial Heat Exchanger Internals Structure for Fischer-Tropsch (FT) Synthesis — ***Hayder Al-Naseri***, *Joshua P. Schlegel, Muthanna Al-Dahhan*

Paper 234v: Role of Bifurcation Geometry on Stability of Thrombus — ***Hari Hara Sudhan Lakshmanan***, *Jeevan Maddala*

Paper 234w: Using μ²rheology to Measure Rheological Properties of Hydrogenated Castor Oil — ***Matthew Wehrman***, *Seth Lindberg, Kelly M. Schultz*

Paper 234z: Deposition and Oil-Brine Interfacial Rheology of Asphaltene-Stabilized Emulsions — ***Yu-Jiun Lin***, *Peng He, Zhuqing Zhang, Steve Kuei, Sibani Lisa Biswal*

■ TURBULENT & REACTIVE FLOWS

Paper 234x: CFD Simulation of Bubble Columns Operating in Heterogeneous Regime — *Tatiana Matiazzo, Bruna L. Mees, Jaci C. S. C. Bastos, Henry F. Meier,* ***Marcela Kotsuka Silva***

Paper 234y: Stability of Stagnation-Point Flows of Newtonian and Complex Fluids — *Noa Burshtein, Simon Haward,* ***Amy Shen***

(235) Rapid Development and Implementation of Bioseparations
Monday, Oct 30, 3:15 PM
MCC, M100D

Alpana Naresh, Chair
Ronald Michalsky, Co-Chair

Sponsored by: Bio Separations

3:15 Paper 235a: Nanostructured Redox Interfaces for Electrochemically Mediated Bioseparations — ***Xiao Su***, *Jonas Huebner, Matthias Franzreb, Timothy Jamison, T. Alan Hatton*

3:35 Paper 235b: Breaking Through the Limits of Chromatography Operations: Integration of a Novel Modular Chromatography Scaffold with Bed Design Features to Achieve High Speed and High Productivity — ***Marty Siwak***

4:00 Paper 235c: Multi-Column Continuous Chromatography for Process-Intensified Capture and Polishing of Monoclonal Antibodies — ***Anthony Grabski***, *William Wessel, Tom Van Oosbree, Emily Schirmer, Robert Mierendorf*

4:25 Paper 235d: Improved Chromatographic Distributors Through CFD Modeling — ***Gastón de los Reyes***, *Sean Fitzgibbon*

4:45 Paper 235e: Methods for Optimizing Bio-Chromatography Processes for Repeated Cyclic Operations — *Noriko Yoshimoto,* ***Shuichi Yamamoto***

5:05 Paper 235h: Advective Flow Membrane Chromatography: Utilization of Flow-through Mode for Scalable, Single-Use Downstream mAb Processing — ***Russell Overbeck***, *Xianwen Chen*

5:25 Paper 235g: Development of Tie Lines for Optimization of Porcine Parvovirus Recovery in Aqueous Two-Phase System — ***Pratik Joshi***, *Matthew Weiss, Caryn L. Heldt*

(236) Reaction Kinetics and Transport Fundamentals for Biomass Conversion: Chemical and Catalytic
Monday, Oct 30, 3:15 PM
MCC, 101B

Xianglan Bai, Chair
Justinus Satrio, Co-Chair

Sponsored by: Sustainable Biorefineries

3:15 Paper 236a: A DEM Modeling of Biomass Fast Pyrolysis in a Double-Screw Reactor — ***Fenglei Qi***, ***Mark Mba Wright***

3:36 Break

3:57 Paper 236c: Modeling and Simulation of a Biphasic Reactor for Upgrading Biofuel Products from Fast Pyrolysis of Biomass: A Mass Transfer Approach — ***Menelik Negash***

4:18 Paper 236d: Hydrocarbon Produced from Upgrading Rich Phenolic Compound Bio-Oil with Low Catalyst Coking — ***Yi Wei***, *Jianbing Ji*

4:39 Paper 236e: Hydrotreating of Catalytic Pyrolysis Oils — ***Kristiina Iisa***, *Kellene Orton, Richard J. French*

5:00 Paper 236f: Renewable Hydrocarbon Production from Catalytic Upgrading of Fast-Pyrolysis Bio-Oil from a Feedstock Blend — ***Mariefel V. Olarte***, *Asanga B. Padmaperuma, Earl Christensen, Jack Ferrell, Gary G. Neuenschwander, Leslie Rotness, Alan H. Zacher, Rafal Gieleciak, Anton Alvarez-Majmutov, Jinwen Chen*

5:21 Paper 236g: CFD-DEM Model for Predicting Producer Gas Contaminants During Biomass Gasification — ***Oluwafemi Oyedeji***, *Norredine Abdoulmoumine*

(237) Reaction Path Analysis II
Monday, Oct 30, 3:15 PM
MCC, L100E

Preetinder Virk, Chair
Michael T. Klein, Co-Chair
Amrit Jalan, Co-Chair
Andrew J. Adamczyk, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

3:15 Paper 237a: Mechanism and Kinetics of Direct Acylation of Furanic and Phenolic Species with Carboxylic Acids — *Abhishek Gumidyala, Bin Wang,* ***Steven Crossley***

3:34 Paper 237b: Approaches and Software Tools for the Development of Molecular-Level Kinetic Mega Models — ***Juan Lucio-Vega***, *Michael T. Klein*

3:53 Paper 237c: First-Principles Insights into the Selective Conversion of Glycerol to 1,3-Propanediol: The Synergistic Effect of Metal and Metal Oxide — ***Jithin John Varghese***, *Liwei Cao, Alexei Lapkin, Yanhui Yang, Samir H. Mushrif*

4:12 Paper 237d: Reaction Mechanism of Glycerol Oxidation to 1,3-Dihydroxyacetone and Glyceraldehyde on Pt Catalyst: A Density Functional Theory Study — ***Hao Yan***, *Xin Jin, Feng Xiang, Yibin Liu, Chaohe Yang*

4:31 Paper 237e: Reaction Network and Mechanistic Assessment of Acrolein Oxidation on an Industrial Oxide Catalyst — ***Jacob Miller***, *Aditya Bhan*

4:50 Paper 237f: The Mechanism of Isobutylene Polymerization: New Insight into Proton-Catalyzed Polymerizations — ***Minh Nguyen Vo***, *Yasemin Basdogan, Bridget Derksen, John A. Keith, Nico Proust, G. Adam Cox, Cliff Kowall, J. Karl Johnson*

5:09 Paper 237g: Unifying Mechanistic Analysis of the Primary Factors Controlling Selectivity in Fructose Dehydration by Acid Catalysts — ***Glen Svenningsen Jr.***, *Rajeev Kumar, Charles Wyman, Phillip Christopher*

5:28 Paper 237h: Reaction Coupling of Nitrobenzene Hydrogenation with Ethylbenzene Dehydrogenation: Reaction Pathways and Kinetics — ***Peng Yu***, *Hsi-Wu Wong*

(238) Research Frontier of Water Sustainability
Monday, Oct 30, 3:15 PM
MCC, 103B

Lan Ying Jiang, Chair
Yunfa Chen, Co-Chair
Tai-Shung Chung, Co-Chair

Sponsored by: Innovations of Green Process Engineering for Sustainable Energy and Environment

3:15 Paper 238a: *Porphyridium cruentum* Grown on Swine Waste has Minimal Changes to Its Fatty Acid Composition — ***Humeyra B. Ulusoy Erol***, *Mariana Lara Menegazzo, Emily Gottberg, Jessica Vaden, Maryam Asgharpour, Christa N. Hestekin, Jamie A. Hestekin*

3:37 Paper 238b: Granulation of Anammox Sludge in Upflow Reactors — ***Chong-Jian Tang***

3:59 Paper 238c Using a Bio-Derived Solvent to Cast Polysulfone Ultrafiltration Membranes — *Xiaobo Dong,* ***Sneha Chede***, *Isabel Escobar*

4:21 Paper 238d: Reducing Specific Energy Consumption of Seawater Desalination: Staged RO or RO-PRO? — ***Mingheng Li***

4:43 Paper 238e: Novel Thin-Film Composite Nanofiltration Membrane Prepared with Ethylenediamine-Functionalized β-Cyclodextrin for Water Treatment — ***Shu Xiong***, *Yan Wang*

5:05 Paper 238f: Concentration of Titania Waste Acid by Direct-Contact Membrane Distillation: Influence of Ferrous Sulfate and Polyacrylamide on Flux and Rejection — ***Lan Ying Jiang***

5:27 Paper 238g: Molecular Interaction Between Acidic sPPSU and Basic HPEI Polymers and Its Effects on Membrane Formation for Ultrafiltration — ***Lin Luo***, *Tai-Shung Chung, Martin Weber, Claudia Staudt, Christian Maletzko*

(239) Solids Handling and Processing I
Monday, Oct 30, 3:15 PM
MCC, 200J

Kerry Johanson, Chair
Madhusudhan Kodam, Co-Chair

Sponsored by: Solids Flow, Handling and Processing

3:15 Paper 239a: Discrete and Continuum Plane-Hopper Flow Simulations with Experimental Validation Using X-Ray Imaging, Arch Profilometry, and Wall Pressure Measurements — ***Tyler L. Westover***, *Kunal Pardikar, Yidong Xia, Jordan Klinger, Sergio Hernandez, Glen Monson, Hai Huang, Carl R. Wassgren*

3:33 Paper 239b: Predicting Feeder Performance During Hopper Refill Based on Material Flow Properties — ***Tianyi Li***, *Yifan Wang, Benjamin Glasser, Fernando Muzzio*

3:51 Paper 239c: Transfer Chute Design Considerations for Dust Control Using Computational Fluid Dynamics (CFD) — ***Xiaoling Chen***, *Craig Wheeler*

4:09 Paper 239d: Development of an Empirical Model to Predict the Mean Residence Time in a Tablet Press Feeder — ***Nobel O. Sierra-Vega***, *Rafael Mendez-Roman*

4:27 Paper 239e: Effect of Baffles on Heat Transfer and Temperature Distribution in Granular Materials in Rotating Drums — ***Bereket Yohannes***, *Meghana Kalluri, William G. Borghard, F. Muzzio, Benjamin Glasser, Alberto M. Cuitino*

4:45 Paper 239f: Modeling of the Flow Dynamics of High-Porosity Filter Media in Depth Filtration — ***Siying Zhang***, *Xavier Strittmatter, Joseph J. McCarthy*

5:03 Paper 239g: Drying Behaviour of Complex Amorphous Solids — ***Daryl Williams***

5:21 Paper 239h: Effect of Particle Surface Roughness on Wall-to-Particle Heat Transfer — ***Ipsita Mishra***, *Casey Q. LaMarche, Aaron Lattanzi, Aaron Morris, Christine M. Hrenya*

(240) Solve This! Fundamental Approach to Problem Solving in Industrial Processes II (Invited Talks)
Monday, Oct 30, 3:15 PM
MCC, 101I

Zdravko Stefanov, Chair
Paul Chauvel, Jr., Co-Chair
Eldad Herceg, Co-Chair
Dana A. Livingston, Co-Chair

Sponsored by: Young Professionals Committee (YPC)

3:15 Paper 240a: Solve this! Fundamental Approach to Problem Solving in Industrial Processes II (Invited Talks) — ***Zdravko Stefanov, Paul Chauvel, Jr., Eldad Herceg, Dana A. Livingston***

(241) Topical Plenary: Advances in Biosensing (Invited Talks)
Monday, Oct 30, 3:15 PM
MCC, M100A

Andrew P. Goodwin, Chair
Hadley D. Sikes, Co-Chair
Brad Berron, Co-Chair

Sponsored by: Sensors

3:15 Paper 241a: Principles for Biosensing Based on Liquid Crystals — ***Nicholas L. Abbott***

3:50 Paper 241b: In Search of an In-Vivo Biopsy: Studies in Stimulus-Responsive Colloids for Biosensing — ***Andrew P. Goodwin***

4:25 Paper 241c: Printed Electronic Biosensors for Protein Detection — ***Kevin D. Dorfman***

5:00 Paper 241d: Nanostructures for Biosensing — ***Sang-Hyun Oh***

(242) Unconventionals: Shale Oil, Oil Sands and Other Heavy Fuels
Monday, Oct 30, 3:15 PM
MCC, 200A

Paul M. Mathias, Chair
Wang Shu, Co-Chair

Sponsored by: Alternate Fuels and New Technology

3:15 Paper 242a: Mitigating Risks for Refiners Processing Opportunity Crudes — ***Tim Olsen***

3:34 Paper 242b: Asphaltene Precipitation in Bitumen-Diluent Blends — ***Wattana Chaisoontornyotin***, *Yuan Yang, Jingzhou Zhang, Samson Ng, Michael P. Hoepfner*

3:53 Paper 242c: CFD Applied to Shale Oil Pyrolysis — *Carina Stahnke, Marcela Kotsuka Silva, Leonardo M. Rosa, Dirceu Noriler, Henry F. Meier,* ***Jaci Carlo Schramm Camara Bastos***

4:12 Paper 242d: Future Oil Sands Production Costs and GHG Emissions Based on Emerging Technologies — ***Experience I. Nduagu***, *Alpha Sow, Evar Umeozor, Dinara Millington*

4:31 Paper 242e: Impact of Opportunity Crudes on Desalter Operation and Wastewater Treatment Performance in a Refinery — ***Somnath Basu***

4:50 Paper 242f: A Tool for Understanding Foaming Tendencies, Coke Morphology, and Quench Effectiveness: Real-Time Visualization into Pilot Delayed-Coker Drum — ***Amaka Waturuocha***, *Dwijen Banerjee, Michael Volk, Glixon Mavarez Nava, Keith Wisecarver*

5:09 Paper 242g: Shale Oil as Steam Cracking Feedstock: GC × GC Characterization and COILSIM1D Modeling — ***Nenad D. Ristic***, *Marko R. Djokic, Ismaël Amghizar, Kevin M. Van Geem, Guy B. Marin*

5:28 Paper 242h: Characteristics of Unconventional and Heavy Oils: Their Economic and Environmental Impacts in Production and Processing — ***M. R. Riazi***

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(243) Use the FE Exam as an Assessment Tool?
Monday, Oct 30, 3:15 PM
MCC, L100G

William Parrish, Chair
John Wagner, Co-Chair

Sponsored by:
Professional Development

3:15 Paper 243a: Introduction — ***William R. Parrish***

3:20 Paper 243b: Using the FE Exam as an Outcome Assessment Tool — ***David Whitman***

4:05 Paper 243c: Panelist Background and Introductory Remarks for Professor Wagner — ***John Wagner***

4:15 Paper 243d: Panelist Background and Brief Views of Professor Bullard — ***Lisa G. Bullard***

4:25 Paper 243e: Panelist Background and Brief Remarks for Professor Silverstein — ***David Silverstein***

4:35 Panel Discussion

5:35 Paper 243f: Session Summary — ***John Wagner***

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(244) Electrokinetics and Microfluidics for Biomolecular Analysis
Monday, Oct 30, 3:30 PM
Hilton, Marquette IV/V/VI/VII

David Charlot, Chair
Shubha Tiwari, Co-Chair

Sponsored by:
2017 Annual Meeting of the AES Electrophoresis Society

3:30 Paper 244a: Entropic Trap-Based Tunable Short-Pass Filter to Recover Long DNA for Genomic Applications — ***Pranav Agrawal***, *Zsófia Bognár, Kevin D. Dorfman*

3:45 Paper 244b: Dielectrophoretic Quantification of Mixed Blood Populations for Detection of Autologous Blood Transfusions — ***Francesca Crivellari***, *Nicholas Mavrogiannis, Zachary R. Gagnon*

4:00 Paper 244c: Non-Optical Biomolecular Detection in Human Serum Using Interfacial Electrokinetic Transduction — ***Nicholas Mavrogiannis***, *Zachary R. Gagnon*

4:15 Paper 244d: Pulsed-Field Electrophoresis for Microfluidic Devices — ***Guiren Wang***, *Xin Liu, Travis Stewart*

4:30 Paper 244e: Low-Loss On-Chip Sample Pretreatment: Depletion Isotachophoretic Isolation of DNAs from Inhibitor-Rich Samples by an Ionic Transistor — *Gongchen Sun,* ***Chenguang Zhang,*** *Satyajyoti Senapati, Hsueh-Chia Chang*

4:45 Paper 244f: Plasmonic ELISA Biosensor with Tunable Sensitivity and Selectivity — ***Andrew House***, *Natalija Tasovac, Ridhi Mehta, K. Stephen Suh, Sagnik Basuray*

5:00 Paper 244g: Modeling and Validation of the Effect of Electric Field on Drug Delivery into the Tumor Cell — ***Maryam Moarefian***, ***Luke E. K. Achenie***

5:15 Paper 244h: A Shear-Enhanced CNT-DEP Nanosensor Platform for Single-Cell Protein Assay — ***Diya Li, Satyajyoti Senapati***, *Siyuan Zhang, Hsueh -Chia Chang*

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(245) Solvent Extraction and Adsorption in Spent Fuel Reprocessing and Radioactive Waste Management
Monday, Oct 30, 4:00 PM
MCC, 200D

Jack D. Law, Chair
Kevin Lyon, Co-Chair

Sponsored by:
Nuclear Engineering Division

4:00 Paper 245a: The Preparation of Titanate Nano-Materials Removing Efficiently Cs-137 from Radioactive Waste Water — ***Dejun Liu***, *Jing Fu, Rong Zhang, Ning Ma, Tian Luo*

4:25 Paper 245b: Aging Processes of Ag-Exchanged Mordenite and Ag-Functionalized Silica Aerogel in Spent Nuclear Fuel Reprocessing Off-Gases — ***Yue Nan***, *Abney Carter, Seungrag Choi, Jiuxu Liu, Lawrence L. Tavlarides*

4:50 Paper 245c: Adsorption Modeling for Selective Capture of Uranium from Seawater — ***Austin Ladshaw***, *Sotira Yiacoumi, Costas Tsouris*

5:15 Paper 245d: Selective Adsorption for Kr/Xe Capture and Separation — ***Amy Welty***, *Mitchell Greenhalgh, Troy G. Garn*

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(246) CAST Rapid-Fire Session I
Monday, Oct 30, 4:45 PM
MCC, 103C

Kyle V. Camarda, Chair
Prodromos Daoutidis, Co-Chair

Sponsored by:
Computing Systems and Technology Division

3:15 Paper 246a: A Simultaneous Utility and Area Targeting Model for Integrated Process and Heat-Exchanger Network Synthesis — ***Lingxun Kong***, *Christos T. Maravelias*

3:15 Paper 246b: The Design of Beta Amino Acid Fragments to Inhibit the Aggregation of Alpha Synuclein — ***Rex Gaumer,*** *Matthew Hartenstein, Kyle V. Camarda*

3:15 Paper 246c: Sustainable and Efficient CO_2 Utilization: Production of Dimethyl Carbonate by an Indirect Route Using Ethylene Oxide and Methanol — ***Adem R. N. Aouichaoui***, ***Anders J. S. Olsen***, ***Kevin C. Feldmann***, *Spardha Jhamb*

3:15 Paper 246d: Superstructure Formulation and Optimization of a Methane-Based Chemical Refinery for Co-Producing Olefins and Aromatics — ***Zhihong Yuan***

3:15 Paper 246e: A Mindset Change from Batch to Continuous Pharmaceutical Crystallization Process Control: The Residence Time–Based Feedback Control — ***Qinglin Su***, *Zoltan K. Nagy*

3:15 Paper 246f: Computational Evaluation of the Performance of Three Treatment Chamber Designs for Electric-Field-Assisted Microbial Inactivation Process — ***Hassan Masood***, *Patrick J. Cullen, Francisco J. Trujillo*

3:15 Paper 246g: Biochemical Process Design: The Sustainable Production of Biobutanol from Wheat Straw Using *Clostridium acetobutylicum* — ***Andreas Norgreen***, ***Caroline Norgreen***, ***Christina Etler***, *Olivia Ana Perederic*

3:15 Paper 246h: Probabilistic Process Design Under Uncertainty via Dynamic Optimization — ***Calvin Tsay***, *Richard Pattison, Michael Baldea*

3:15 Paper 246i: A Superstructure-Based Assessment Framework for Downstream Bio-Separation — ***Wenzhao (Tony) Wu***, *Kirti Maheshkumar Yenkie, Christos T. Maravelias*

3:15 Paper 246j: CFD Modeling of Piston-Type Direct Work Exchangers — ***Aida Amini Rankouhi***, *Yinlun Huang*

3:15 Paper 246k: Simultaneous Process Synthesis and Heat Integration Using a Single Superstructure — ***Salih E. Demirel***, *Jianping Li, M. M. Faruque Hasan*

5:40 Paper 246l: Mosaic: Parallel Computing, Multi-Objective Optimization Applications — ***Bridgette Befort***, *Kyle V. Camarda*

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(247) CAST Rapid-Fire Session II
Monday, Oct 30, 4:45 PM
MCC, 103D

Sujit S. Jogwar, Chair
Prodromos Daoutidis, Co-Chair

Sponsored by:
Computing Systems and Technology Division

3:15 Paper 188n: Computation of Terminal Constraints for Large-Scale NMPC — ***Devin Griffith***, *Lorenz T. Biegler*

3:15 Paper 186m: Physically Based Dynamic Modeling for Predictive Simulation of a Net-Zero Home — *Alan Uy,* ***Raymond Adomaitis***

3:15 Paper 188y: Nonlinear System Identification and Dynamic Real-Time Optimization of Postcombustion CO_2 Capture Processes for Cycling Applications — ***Rebecca Kim***, *Fernando V. Lima*

3:15 Paper 188h: Strategies for Minimum-Variance ALS Estimation of Noise Covariance Matrices — ***Travis J. Arnold***, *James B. Rawlings*

3:15 Paper 188aa: Uniting Lyapunov-Based MPC with Closed-Loop Subspace Identification — ***Masoud Kheradmandi***, *Prashant Mhaskar*

3:15 Paper 188k: Optimal Operation of Heat Exchanger Networks Through Heat Duty Redistribution Using Energy Flow Graphs — ***Sujit S. Jogwar***

3:15 Paper 188m: A Multi-Parametric Bi-Level Optimization Strategy for Hierarchical Model Predictive Control — ***Styliani Avraamidou***, *Nikolaos A. Diangelakis, Efstratios N. Pistikopoulos*

3:15 Paper 188w: Data-Driven Modeling and Optimization of an Ethane Steam Cracker — ***Burcu Beykal,*** *Onur Onel, Efstratios N. Pistikopoulos*

3:15 Paper 188c: Development of Biomimetic Approaches for Intelligent Control System Design, Monitoring and Optimization of Advanced Energy Systems — *Temitayo Bankole, Gaurav V. Mirlekar, Ghassan Al-Sinbol, Berhane Gebreslassie, Fernando V. Lima, Mario Perhinschi, Urmila M. Diwekar, Richard Turton,* ***Debangsu Bhattacharyya***

3:15 Paper 188b: Fractional Order Plus Time Delay Model Extending the First Order Plus Time Delay Model — ***Yongjeh Lee***, *Dae Ryook Yang, Jietae Lee, Thomas F. Edgar*

3:15 Paper 188r: A Case Study on Semi-Batch Endpoint Control — ***Nishith R. Patel***, *James B. Rawlings*

3:15 Paper 188d: Non-Intrusive Appliance Load Monitoring Algorithm to Detect Simultaneous State Changes of Electrical Appliances — ***Nikita Patel***, *Babji Srinivasan,* ***Rajagopalan Srinivasan***

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(248) CAST Rapid-Fire Session III
Monday, Oct 30, 4:45 PM
MCC, 103E

Debangsu Bhattacharyya, Chair
Prodromos Daoutidis, Co-Chair

Sponsored by:
Computing Systems and Technology Division

3:15 Paper 189g: Sustainable CO_2 Utilization in DMC Production — ***Bjartur Jacobsen, Frederikke Zilstorff***

3:15 Paper 188v: Closed-Loop Re-Identification of Multi-Rate System Using N4SID and Zone MPC — ***ByungJun Park***, *Se-Kyu Oh, Jong Min Lee*

3:15 Paper 187b: Evaluating Hospital Performance Using Process Systems Engineering Tools — ***Jangwon Lee***, *Ravi Chinta, Q. Peter He*

3:15 Paper 188p: A Biologically Inspired Optimal Control Framework: Application to the Hybrid Performance (HyPer) System — ***Gaurav V. Mirlekar***, *Paolo Pezzini, Kenneth M. Bryden, David Tucker, Fernando V. Lima*

3:15 Paper 189n: A Systematic Process Design for Sustainable Dimethyl Carbonate Production Through Carbon Dioxide Utilization — ***Jeska Naujoks***, ***Shwetha Meena Sakthi Nallasivam***, ***Niranchana Venkatesh***, *Spardha Jhamb*

3:15 Paper 189o: Evaluation of Carbon Monetization in Power Systems for Flaring Mitigation — ***Javier Tovar-Facio***, *Luis Fabian Fuentes-Cortes, José María Ponce-Ortega*

3:15 Paper 190c: Optimal Control Structure Design for Cyber-Physical Systems — ***Temitayo Bankole***, *Paolo Pezzini, Nor Farida, Kenneth M. Bryden, David Tucker, Debangsu Bhattacharyya*

3:15 Paper 190t: Bilevel Optimization Strategies to Couple Production of Biotechnological Products with Growth in Cyanobacteria — *Romina Lasry Testa, Claudio Delpino, Vanina Estrada,* ***Maria Soledad Diaz***

3:15 Paper 190f: Dynamic Modeling and Control of a Natural Gas Combined Cycle (NGCC) Power Plant Integrated with CO_2 Capture — ***Yifan Wang***, *Debangsu Bhattacharyya, Richard Turton*

3:15 Paper 190s: An Optimization Approach to Ordinary-Fractional Multi-Compartmental Models with Applications to Pharmacokinetics and Optimal Drug Usage — ***Vicente Rico-Ramirez***, *Julio C. Barrera-Martinez, Edgar O. Castrejon-Gonzalez, Edna S. Lopez-Saucedo*

3:15 Paper 189ab: An Efficient Approach to Bounding Multistage Stochastic Programs Using Sample Average Approximation — ***Katie Martin***, *Brianna Christian, Selen Cremaschi*

3:15 Paper 186g: Novel Non-Invasive Quantification of Coronary Artery Stenosis — ***Javad Hashemi***, *Shahab Ghafghazi, R. Eric Berson*

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(249) CAST Rapid-Fire Session IV
Monday, Oct 30, 4:45 PM
MCC, 103F

Q. Peter He, Chair
Prodromos Daoutidis, Co-Chair

Sponsored by:
Computing Systems and Technology Division

3:15 Paper 186a: A Minimalist Model for Rapid Simulation Enabling Optimization of the Uniformity of Multiple Simultaneous Hydraulic Fracture Growth — ***Cheng Cheng***, *Andrew P. Bunger*

3:15 Paper 187i: An Inverse-Model-Based Methodology for Real-Time Fault Diagnosis in Non-Square Multivariate Dynamic Systems — ***Liwen Chen***, *Qiang Xu*

3:15 Paper 186n: Comparison of Various Techniques for Solving Complex Chemical Equilibrium Problems — ***Mordechai Shacham***, *Neima Brauner*

3:15 Paper 187d: Multiscale Dynamics System Identification of Time Series of Riser Reactor Temperature in FCC Process Based on Hilbert-Huang Transform — ***Daofan Cao***, *Yingya Wu, Xingying Lan, Jinsen Gao, Chunming Xu*

3:15 Paper 186e: A Two-Phase Imbibition-Drainage Model for Soils Amended with Biochars — ***Yi Chen***, *Kyriacos Zygourakis*

3:15 Paper 187k: Time-Frequency Analysis of Pupillary Fluctuations to Monitor Control Room Operators During Plant Abnormalities — ***Punitkumar Bhavsar***, *Babji Srinivasan,* ***Rajagopalan Srinivasan***

3:15 Paper 187g: Plant-Wide Visualization for Situation Awareness Using Ising Model-Based Clustering of Vanishing Correlations — ***Masanao Natsumeda***

3:15 Paper 189q: Development of Reaction Mechanism and Kinetics for the Production of Butadiene Through Oxidative Dehydrogenation of Alkane or Alkene — ***Junghoon Kim***, *Sungwon Hwang*

3:15 Paper 187c: DeepMetabolism: A Deep Learning Algorithm to Predict Phenotype from Genome Sequencing — ***Weihua Guo***, *You Xu, Xueyang Feng*

3:15 Paper 186j: Theoretical Analysis and Process Design for Dual-Impinging Jet Cooling Crystallization — ***Mo Jiang***, *J. Carl Pirkle Jr., Richard D. Braatz*

3:15 Paper 186d: Quenched Periodic Extension for Interpolation Using Radial Basis Functions — ***Rafael G. Henríquez Rivera***, *Ludwig C. Nitsche*

3:15 Paper 187e: Next-Generation Process Monitoring for IoT-Enabled Smart Manufacturing — ***Q. Peter He***, *Jin Wang*

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(250) Poster Session: AES
Monday, Oct 30, 6:00 PM
Hilton, Marquette IV/V/VI/VII

Blanca H. Lapizco-Encinas, Chair
Victor M. Ugaz, Co-Chair

Sponsored by:
2017 Annual Meeting of the AES Electrophoresis Society

Paper 250a: Flow-Regulated Anodic Growth of TiO_2 Nanotubes in Microfluidics — *Rong Fan, Xinye Chen, Zihao Wang, David Custer,* ***Jiandi Wan***

Paper 250b: Dielectrophoretic Separation of Large Microscale Particles (dp>5 um) by Exploiting Charge Differences — ***Danielle Polniak***, *Eric Goodrich, Blanca H. Lapizco-Encinas*

Paper 250c: Dielectrophoretic Assessment of Sub-Micron Particles by Exploiting Charge Differences — ***Eric Goodrich***, *Maria Romero-Creel, Danielle Polniak, Blanca H. Lapizco-Encinas*

Paper 250d: Research of DNA Separation by Post Array Under Intermittent Electric Field — ***Chih-Hsiang Shu***, *Sheng-Hung Wang, Chen-Ju Liu, Chih-Chen Hsieh*

Paper 250e: Insight into Coal Structure Based on Benzene Carboxylic Acids from the Coal via Oxidation — *Fan Yang, Yucui Hou, Muge Niu, Shuhang Ren,* ***Weize Wu***

Paper 250f: Multiphysics Modeling of Microfluidic Device to Investigate the Effect of Electric Field on Drug Delivery into the Tumor Cell — ***Maryam Moarefian***, ***Luke E. K. Achenie***

Paper 250g: NVU-on-a-Chip: Optimizing Brain Endothelial Cell Culture for Microfluidic Modeling of the NVU — ***Victoria Harbour,*** *Bhuvana Mohanlal, Samuel Roy, Sagnik Basuray*

Paper 250h: Electrohydrodynamic Scaling Laws Analysis in a Microfluidic IsoDep Device — ***Mohamed Rashed***

Paper 250i: Fundamentals, Calibration and Preliminary Results Using the DSC Technique for Hydrogel Thermoporometry — ***Anfal Haris***, *J. Robby Sanders, Pedro E. Arce, Joseph J. Biernacki*

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(251) Pharmaceutical Discovery, Development, and Manufacturing Forum Awards Ceremony
Monday, Oct 30, 6:30 PM
MCC, 205A/B

Zoltan K. Nagy, Chair

Sponsored by:
Pharmaceutical Discovery, Development and Manufacturing Forum

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(252) 3D Printing Fundamentals and Applications
Tuesday, Oct 31, 8:00 AM
MCC, 101A

Nima Yazdanpanah, Chair
Lin Li, Co-Chair

Sponsored by:
Next-Gen Manufacturing

8:00 Paper 252c: The Potential and Challenges of Multifunctional 3D Printing — ***Denis Cormier***

8:30 Paper 252a: Applications of Desktop 3D Printing in the Biopharmaceutical Industry — ***Adam Procopio***, *Derrick Smith, Yash Kapoor, Ashley Johnson, Seth Forster, Andre Hermans, Tiffany Gustafson*

9:00 Paper 252b: Three-Dimensional Printing via "Capillary Engineering" of Multiphasic Elastomer Inks — *Sangchul Roh*, ***Orlin D. Velev***

9:30 Paper 252d: Advancing Diagnostics and Therapies by Enabling Scientists with 3D-Printing Technologies — ***Dana Spence***

10:00 Paper 252e: Perfusion Directed 3D Bone Mineralization Using Custom-Modified 3D Printers — ***Pranav Soman***

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(253) Adsorbent Materials
Tuesday, Oct 31, 8:00 AM
MCC, M100E

Dipendu Saha, Chair
Roger D. Whitley, Co-Chair

Sponsored by:
Adsorption and Ion Exchange

8:00 Paper 253a: Direct Synthesis and Tuning of Highly Porous Boron Nitride: Towards a New Class of Adsorbent — ***Sofia Marchesini***, *Catriona M. McGilvery, Josh Bailey, Camille Petit*

8:20 Paper 253b: Exploiting Unique Properties of Porous Polymers for Air Pollution Control — ***Mohsen Ghafari***, *John D. Atkinson*

8:40 Paper 253c: Developing Nanometal Oxide Composite from Solid Waste to Make an Efficient Adsorbent for Heavy Metal Removal — ***Aditi Chatterjee***, *Amiya Kumar Jana, Jayanta Kumar Basu*

9:00 Paper 253d: Ionic Liquids and Ionic Liquid-Functionalized Carbons for Sorption of Gaseous Toxins — ***Elizabeth J. Biddinger***, *Devin Peck, Krishnakoli Adhikary*

9:20 Paper 253e: Preparation and Its Excellent $CO_2/CH_4/N_2$ Adsorption Selectivity of Novel Glucose-Based Adsorbents (C-GLC) with High-BET Surface Area — ***Xingjie Wang***, *Binqin Yuan, Xin Zhou, Qibin Xia,* ***Zhong Li***

9:40 Paper 253f: Hybrid of Metal-Organic Framework and Ionic Liquid as Adsorbent for Adsorptive Separation of Acetylene and Ethylene — ***Zongbi Bao***

10:00 Paper 253g: Binary Gas Adsorption Equilibria on MIL-53(Al) — ***Sasidhar Gumma***, *Kara Ufuoma, Orhan Talu*

(254) Advances in Computational Methods and Numerical Analysis
Tuesday, Oct 31, 8:00 AM
MCC, 103F

Jinfeng Liu, Chair
Kamil Ahmad Khan, Co-Chair
Martin Guay, Co-Chair

Sponsored by:
Applied Mathematics and Numerical Analysis

8:00 Paper 254a: GPU Parameter Tuning for Dense Linear Least Squares Problems — ***Benjamin Sauk***, *Nikolaos Ploskas, Nick Sahinidis*

8:21 Paper 254b: Phase Change Transient Model for Predicting Frost Formation in Ambient Air Vaporizer — ***Jongmin Park***, *Yongkyu Lee, Jonggeol Na, Chonghun Han, Wonbo Lee*

8:42 Paper 254c: Simulation of the Effect of Contact Area Loss in All-Solid-State Batteries — ***Hong-Kang Tian***, *Yue Qi*

9:03 Paper 254d: Multi-Phase Mathematical Modeling of Compressed CO_2 Expansion Through a Coanda Nozzle — *Odell Glenn Jr., Sirivatch Shimpalee,* ***Michael A. Matthews***

9:24 Paper 254e: Stochastic Modeling of CTB-GM1 Binding Mechanisms — ***Dongheon Lee,*** *John Larry Dial III, Joseph Sangil Kwon, Singla Akshi, Hung-Jen Wu*

9:45 Paper 254f: Numerical Investigation of a Water Droplet on Vibrating Surface with and Without Inclination — ***Ping He***, *Chun-Wei Yao*

10:06 Paper 254g: Novel Optimization-Based Adaptive Sparse-Grid Methods for Numerical Integration — ***Chris A. Kieslich***, *Fani Boukouvala*

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(255) Advances in Data Analysis, Information Management, and Intelligent Systems I
Tuesday, Oct 31, 8:00 AM
MCC, 103E

Fani Boukouvala, Chair
Franjo Cecelja, Co-Chair

Sponsored by:
Data and Information Systems

8:00 Paper 255a: Comparison of Machine Learning Approaches for Process Model Development from Big Data — ***Sarah Davis***, *Selen Cremaschi, Mario Richard Eden*

8:19 Paper 255b: Application of Machine Learning Algorithms for the Selection of Jet Fuel from Hydrocarbon Blends — ***Rajib Mukherjee***, *Noof Abdalla, Nasr Mohamed, Marwan El Wahsh, Nimir El-bashir, Mahmoud M. El-Halwagi*

8:38 Paper 255c: Building Deep Learning–Based Predictive Model and Advisory Control System for a Blast Furnace Operation — ***Young M. Lee***, *Kyongmin Yeo, Nam Nguyen, Igor Melnyk, Jayant Kalagnanam, Seho Choi, Yong-Soo Kim, Kyung-Lyong Han*

8:57 Paper 255d: Determination of the Optimal Number of Eigenfunctions in Proper Orthogonal Decomposition Based on Machine Learning — ***Harwinder Singh Sidhu***, *Abhinav Narasingam, Prashanth Siddhamshetty, Joseph Sangil Kwon*

9:16 Paper 255e: A Scalable Statistical Machine Learning Method: Application for Fault Detection and Fault Propagation Pattern Inference in the Tennessee Eastman Process — *Taha Mohseni Ahooyi, Jeffrey E. Arbogast,* ***Masoud Soroush***

9:35 Paper 255f: Decision Support Platform for the Automation of Processing Recipes and Process Scheduling Management Supported by Knowledge Management — *Elisabet Capón-García,* ***Edrisi Muñoz, Luis Puigjaner***

9:54 Paper 255g: Machine Learning–Based Uncertainty Quantification of Erosion in Pipeline Transportation — ***Wei Dai***, *Selen Cremaschi*

10:13 Paper 255h: Generating Ontology-Based Process Models Automatically — ***Arne Tobias Elve***, *Heinz A. Preisig*

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(256) Advances in Functional Foods Production
Tuesday, Oct 31, 8:00 AM
MCC, 206A/B

Hesham Ali El-Enshasy, Chair
Nuttha Thongchul, Co-Chair
Dimple Kundiyana, Co-Chair

Sponsored by: Food

8:00 Paper 256a: Optimization of Hyaluronic Acid Production by *Streptococcus zooepidemicus* for Biomedical Applications — ***Nuttha Thongchul***, *Jirabhorn Piluk, Sitanan Thitiprasert*

8:18 Paper 256b: Mathematical Study for Prediction of Shelf Life of Curly Hydroponic Lettuce — *Fernanda Raquel Wust Schmitz, Juscelino Almeida Jr., Lisiane Fernandes de Carvalho, Savio Bertoli,* ***Laércio Ender,*** *Carolina Krebs de Souza*

8:36 Paper 256c: Production of Polymalic Acid (PMA) and Malic Acid from Food Processing Byproducts by *Aureobasidium pullulans* — ***Chi Cheng***, *Shang-Tian Yang*

8:54 Paper 256d: Growth Kinetics and Viability Studies of Common Probiotic Bacteria on Date Syrup — *Marwa Al Farsi,* ***Avnish Pareek***, *Taqi Ahmed Khan, Hesham El-Enshasy*

9:12 Paper 256e: Shape-Changing Food Transforms from 2D to 3D by Water Interaction Through Cooking — ***Wen Wang***, *Lining Yao, Teng Zhang, Chin-Yi Cheng, Daniel Levine, Hiroshi Ishii*

9:30 Paper 256f: Optimization of Growth Media and Functionality Characterization of New Potential Probiotic *L. salivarius*, Isolated from Human Milk — ***Roslinda Abd Malek***, *Solleh Ramli, Hesham El-Enshasy*

9:48 Paper 256g: Application of Microbial Factory Technology to Production of Food Materials — ***Jin-Ho Seo***

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(257) Advances in Process Intensification: Enhanced Mass Transfer
Tuesday, Oct 31, 8:00 AM
MCC, 101E

R. Bruce Eldridge, Chair

Sponsored by:
Process Intensification & Modular Chemical Processing

8:00 Paper 257a: Vapor Recompression Mechanism Introducing in Internal Heat-Integrated Distillation Column: Impact of Internal Energy-Driven Intermediate and Bottom Reboiler — ***Bandaru Kiran***

8:25 Paper 257b: Experimental Studies Controlling Trace Components in a Dividing-Wall Distillation Column — ***Melissa Donahue***, *Michael Baldea, R. Bruce Eldridge*

8:50 Paper 257c: Novel Metal-Enzyme Catalyst for One-Pot Dynamic Resolution in a Spinning Cloth Disc Reactor — ***Parimala Shivaprasad***, *Matthew Jones, Emma Emanuelsson*

9:15 Paper 257d: Scale and Effects of Catalyst Deactivation in Enzymatic Catalyzed Reactive Distillation — ***Torben Egger***, *Georg Fieg*

9:40 Paper 257e: Use of Computational Fluid Dynamics (CFD) Simulation and Image Analysis Tool for Modelling Light in a Microalgal Photobioreactor — ***Arpit Mishra***, ***Geetanjali Yadav***, *Parthasarathi Ghosh, Ramkrishna Sen*

(258) Alternative Fuels Including Biofuels, Hydrogen, Renewable Hydrogen, and Syngas
Tuesday, Oct 31, 8:00 AM
MCC, 200F

Ravi Kolakaluri, Chair
Christopher Tyler, Co-Chair
Cory Jensen, Co-Chair

Sponsored by:
Transport and Energy Processes

8:00 Paper 258a: Insights into the Relationship Between Structure and Reactivity Descriptors in Realistic Nanoparticle Models: A DFT Approach — ***Sumegha Godara***, *Daniela S. Mainardi*

8:25 Paper 258b: Transportation Fuels from Renewable Hydrogen and Green Carbon Dioxide: A Technical, Economic, and Environmental Evaluation — ***Dominik Bongartz***, *Jannik Burre, Sarah Deutz, Larissa Doré, Katharina Eichler, Thomas Grube, Benedikt Heuser, Laura Hombach, Martin Robinius, Luisa Schulze Langenhorst, André Bardow, Stefan Pischinger, Detlef Stolten, Grit Walther, Alexander Mitsos*

8:50 Paper 258c: Hydraulic Retention Time and Temperature Impacts on Biogas Production in Expanded Granular Sludge-Bed Reactor — ***Haider Al-Rubaye***, *Joseph D. Smith, Manohar Manchenahalli, Shruti Karambelkar*

9:15 Paper 258d: Reverse Water-Gas Shift Reaction over Cu-Fe/Al_2O_3 Catalyst in Solid Oxide Electrolysis Cells — ***Qusay Bkour***, *Kai Zhao, Jung-Il Yang, M. Grant Norton, Su Ha*

9:40 Paper 258e: Electrochemical Hydrogenation of Bio-Oil Compounds Using a Polymer Electrolyte Membrane Reactor — ***Chen Li***, *Xiaoyu Zhang, Sandeep Kumar*

10:05 Paper 258f: A Parametric Optimization Study of Downdraft Biomass Gasification Using a Comprehensive Transport and Kinetic Model — ***Tapas Kumar Patra***, *Pratik N. Sheth*

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(259) Applications of Chemical Engineering to Nuclear Materials
Tuesday, Oct 31, 8:00 AM
MCC, 200D

Michael Simpson, Chair

Sponsored by:
Nuclear Engineering Division

8:00 Paper 259a: Continuous Monitoring of Ni Corrosion in Eutectic LiCl-KCl-UCl_3 Using High-Temperature Voltammetry — ***David Horvath,*** *Michael Simpson*

8:22 Paper 259b: A Review of IR Spectroscopic Studies of Molten Fluoride Salts — ***Will B. Derdeyn***, *Ruchi Gakhar, Raluca Scarlat*

8:44 Paper 259c: Effect of LiOH Contamination on the Electrolytic Reduction of Spent Oxide Fuel in Molten LiCl-Li_2O — ***Mario Alberto Gonzalez***, *Michael F. Simpson*

9:06 Paper 259d: Effect of Rotation on Li_2O Entrainment in a Uranium Oxide Reduction Process — ***Adam Burak***, *Michael Simpson*

9:28 Paper 259e: Thermal Conductivity of Tungsten: Effects of Plasma-Related Structural Defects from Molecular-Dynamics Simulation — ***Lin Hu***, *Brian D. Wirth, Dimitrios Maroudas*

9:50 Paper 259f: Visualization of Bubble Dynamics in a Natural-Circulation Boiling Loop — *Swapan Paruya,* ***Jithender Naik L***, *Jyoti Bhati*

10:12 Paper 259g: Effect of Process Parameters on Chlorination of Metallic Rare Earth/Actinide Mixtures — ***Parker Okabe***, *Devin S. Rappleye, Matthew Newton, Michael F. Simpson*

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(260) Applications of Molecular Modeling to Study Interfacial Phenomena
Tuesday, Oct 31, 8:00 AM
MCC, L100H

Jindal K. Shah, Chair
Kevin Hadley, Co-Chair
Jeffrey R. Errington, Co-Chair

Sponsored by:
Computational Molecular Science and Engineering Forum

8:00 Paper 260a: Molecular Investigation into the Transport Across the Blood-Brain Barrier Interface [Invited Talk] — ***Shikha Nangia***, *Flaviyan Jerome Irudayanathan, Nan Wang, Xiaoyi Wang*

8:30 Paper 260b: Adsorption and Self-Assembly of Surfactants on Metallic Surfaces Studied Using Molecular Simulations — ***Sumit Sharma***, *Xueying Ko*

8:45 Paper 260c: Modeling Alkane Partitioning and Phase Behavior on Graphite Pores: A Discussion on Dispersion Free-Energy Formalism — ***Jinlu Liu,*** *Walter G. Chapman*

9:00 Paper 260d: Effect of Solvent on the Binding Energies of Molecules on Metal Surfaces — ***Tonnam Balankura***, *Kristen Fichthorn*

9:15 Paper 260e: Tuning Proximal Water Diffusion via Silanol Patterning on Quartz Surfaces — ***Jacob I. Monroe***, *Alex Schrader, Song-I Han, M. Scott Shell*

9:30 Paper 260f: Molecular Dynamics Studies of the Effects of Ionic Liquid Molecular Properties and Particle Concentration on the Behavior of Nanoparticles at the Ionic Liquid/Water Interface — ***Stella D. Nickerson***, *Lenore L. Dai*

9:45 Paper 260g: Suppression of Capillary Waves in a Dipolar Fluid — ***Jason P. Koski***, *Stan G. Moore, Gary S. Grest, Mark J. Stevens*

10:00 Paper 260h: Evaporation-Induced Nucleation of NaCl in Clay Minerals: Mechanism and Potential Sites — ***Hassan Dashtian***, *Haimeng Wang, Muhammad Sahimi*

10:15 Paper 260i: Computational Investigation of the Role of Topology and Functionalization on ZIF Stability — ***Rebecca Han***, *Souryadeep Bhattacharyya, David Sholl, Sankar Nair*

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(261) Area Plenary: Interfacial Phenomena (Invited Talks)
Tuesday, Oct 31, 8:00 AM
MCC, M100B

Raymond R. Dagastine, Chair
Raymond Tu, Co-Chair

Sponsored by: Interfacial Phenomena

8:00 Paper 261a: Interfacial Dynamics Between Pathogenic Nanoparticles and Cell Membrane Surfaces — ***Susan Daniel***

8:50 Paper 261b: Bicontinuous Microemulsions in Homopolymer-Block Copolymer Blends — ***Frank S. Bates***

9:40 Paper 261c: Self-Assembly of Block Copolymers: From Nanostructure to Function to Applications — ***Paschalis Alexandridis***

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(262) Graduate Student Award Finalists — Area 8E
Tuesday, Oct 31, 8:00 AM
MCC, 211A

Sufei Shi, Chair
James Dorman, Co-Chair

Sponsored by:
Electronics and Photonics

8:00 Paper 262a: Autoperforation of 2D Materials for Generating Two-Terminal Memresistive Janus Particles — ***Albert Tianxiang Liu***, *Pengwei Liu, Michael Strano*

8:15 Paper 262b: Driven Morphological Evolution of Strained Thin-Film Surfaces and Two-Dimensional Materials: Morphological Stability and Pattern Formation — ***Lin Du***, *Dimitrios Maroudas*

8:30 Paper 262c: Optimization of THz-Time Domain Spectroscopy Reflectivity for a 1THz Energy-Harvesting Metamaterial — ***Shendu Yang***, *Zachary Thacker, Evan Allison, Patrick J. Pinhero*

8:45 Paper 262d: Modeling Exciton Dynamics and Low-Frequency Vibrations in Quantum Dot Assemblies — ***Elizabeth M. Y. Lee***, *Adam P. Willard, William A. Tisdale*

9:00 Break

9:25 Paper 262e: Extraordinarily Slow Electron-Hole Recombination in Perovskite-Phase Cesium Lead Iodide — ***Subham Dastidar***, *Siming Li, Jason B. Baxter, Aaron T. Fafarman*

9:40 Paper 262f: Elucidating the Impact of Alcohol Post-Processing in High-Performance Roll-to-Roll Printed Organic Photovoltaics — ***Kevin L. Gu***, *Xiaodan Gu, Hongping Yan, Zhenan Bao*

9:55 Paper 262g: Metamaterial and Rectenna Design and Testing for the Conversion of Blackbody Radiation to Electricity Using 5 THz Devices — ***Evan Allison***, *Zach Thacker, Shendu Yang, Patrick J. Pinhero*

10:10 Paper 262h: Reusable Chromogenic Sensors Enabled by Novel Multi-Stimuli-Responsive Shape Memory Polymers — ***Sin-Yen Leo***, *Peng Jiang*

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(263) Atmospheric Chemistry and Physics I
Tuesday, Oct 31, 8:00 AM
MCC, 102F

Kristina Wagstrom, Chair
Nga Lee Ng, Co-Chair
Shunsuke Nakao, Co-Chair

Sponsored by: Air

8:00 Paper 263a: Gas-Particle Partitioning of Alkyl Nitrates from Anthropogenic Alkanes — ***Dongyu S. Wang***, *Sahil Bhandari, Felipe Cardoso-Saldaña, Surya Venkatesh Dhulipala, Jeff K. Bean, Lea Hildebrandt Ruiz*

8:17 Paper 263b: Why Would Cloud Condensation Nucleus Activity Linearly Change with O/C? Assessing the Role of Volatility, Solubility, and Surface Activity — ***Shunsuke Nakao***

8:34 Paper 263c: Bimodal Aerosol Size Distributions from Laboratory Atomization/Evaporation
— *Hemanta Timsina, Dabrina Dutcher,* ***Timothy Raymond***

8:51 Paper 263d: Oxidized Organic Compounds Formed from Chlorine-Initiated Oxidation of Toluene
— ***Surya Venkatesh Dhulipala****, Lea Hildebrandt Ruiz*

9:08 Paper 263e: Hydrolysis of Organic Nitrates Formed from Oxidation of Biogenic Volatile Organic Compounds
— *Masayuki Takeuchi, Gamze Eris,* ***Nga Lee Ng***

9:25 Paper 263f: Analytical Model for Vapor Condensation on Soot Agglomerates — ***Gennady Gor****, Chao Chen, Alexei Khalizov*

9:42 Paper 263g: Influence of Radioactivity-Induced Charging on Aerosol Interactions — ***Yong-ha Kim****, Sotira Yiacoumi, Athanasios Nenes, Costas Tsouris*

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(264) Biological Conversions and Processes for Renewable Feedstocks
Tuesday, Oct 31, 8:00 AM
MCC, 101B

Hasan K. Atiyeh, Chair
Shishir Chundawat, Co-Chair

Sponsored by:
Sustainable Biorefineries

8:00 Paper 264a: Site-Directed Mutagenesis of Family 64 CBM Provides Insights into the Anomalous Binding Interactions with Pretreated Cellulose During Biomass Saccharification — *Cindy Farino, Bhargava Nemmaru,* ***Shishir P. S. Chundawat***

8:21 Paper 264b: Direct Succinic Acid Production from Non-Hydrolyzed Biomass Using Sequential Solid-State and Slurry Fermentation with Mixed Fungal Cultures — ***Jerico Alcantara****, Logan Hughey, Shaun Shields, Andro Mondala*

8:42 Paper 264c: Enhanced Alcohols, Ketones and Organic Acids Production via Co-Fermentation of Sugars and Gases — ***Hasan K. Atiyeh****, Pradeep Munasinghe, Kan Liu, Ralph S. Tanner, Thaddeus Ezeji*

9:03 Paper 264d: Attainable Region Analysis for Production of Butyl Butyrate via Biochemical Route
— ***Cansu Birgen****, Heinz A. Preisig*

9:24 Paper 264e: Biomass Conversion to Functionalized Carbon
— ***Masoudeh Ahmadi****, Jacek Jasinski, Jagannadh Satyavolu, Mahendra Sunkara*

9:45 Paper 264f: Synthesis of Water-Soluble Oligosaccharides as Potential Prebiotics via Non-Enzymatic Sugar Glycosylation — ***Ning Li****, Zening Wang, Tianjiao Qu, Xuejun Pan*

10:06 Paper 264g: Multiscale Effects of Lignocellulose Bioconversion and Corresponding Process Intensification: From Nanoscale to System Scale
— ***Xuebing Zhao****, Dehua Liu*

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(265) Biomacromolecular Gels
Tuesday, Oct 31, 8:00 AM
MCC, 211B

Muzhou Wang, Chair
Christina Tang, Co-Chair
Samanvaya Srivastava, Co-Chair

Sponsored by: Polymers

8:00 Paper 265a: Allyl Sulfide–Modified Hydrogels with Switchable Properties as Dynamic Cellular Niches
— ***Kristi S. Anseth****, Tobin E. Brown, Joseph Grim, Ian Marozas*

8:30 Paper 265b: Non-Linear Rheology and Fracture in Alginate Hydrogels
— *Seyed Meysam Hashemnejad, Rangana Wijayapala,* ***Santanu Kundu***

8:45 Paper 265c: Analyzing the Effects of Time and Crosslinker Ratio on the Mechanical Properties of Biodegradable Zein Super Gels
— ***Hazal Turasan****, Jozef Kokini*

9:00 Paper 265d: Self-Assembly, Structure and Rheology of Polyelectrolyte Complex Hydrogels
— ***Samanvaya Srivastava****, Adam Levi, Matthew V. Tirrell*

9:15 Paper 265e: Evolution of Mechanics in α-Helix Peptide Bioconjugated Linear- and Star-Block PEG — ***Sean C. O·Neill,*** *Raymond Tu*

9:30 Paper 265f: Modelling of the Degradation of Poly(ethylene glycol)-Co-(lactic acid)-Dimethacrylate Hydrogels — ***Marco Lattuada****, Giuseppe Storti, Vincent Diederich*

9:45 Paper 265g: Tough, Rapidly Swelling Thermoplastic Elastomer Hydrogels for Hemorrhage Control
— ***Erich Bain****, Tyler R. Long, Frederick L. Beyer, Randy A. Mrozek, Joseph L. Lenhart*

10:00 Paper 265h: Synthesis and Characterization of Thermally Responsive N-Isopropylacrylamide Hydrogels Copolymerized with Novel Hydrophobic Polyphenolic Crosslinkers
— ***Shuo Tang****, Thomas Dziubla, J. Zach Hilt*

10:15 Paper 265i: Novel Biocompatible Thermo-Responsive Poly(G-vinyl Caprolactam)/Clay Nanocomposite Hydrogels with Macro-Porous Structure and High Mechanical Property
— ***Zhuang Liu****, Kun Shi, Xiao-Jie Ju, Wei Wang, Rui Xie, Liang-Yin Chu*

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(266) Biomass Characterization, Pretreatment, and Fractionation
Tuesday, Oct 31, 8:00 AM
MCC, 200E

Xuejun Pan, Chair
Justinus Satrio, Co-Chair

Sponsored by:
Biorefinery Technologies for Forest-Based Lignocellulosic Biomass

8:00 Paper 266a: Resonant Soft X-Ray Scattering of Cellulose Microstructure in Plant Cell Walls — *Dan Ye, Sintu Rongpipi, Sarah Kiemle, Cheng Wang, Daniel Cosgrove, Enrique D. Gomez,* ***Esther W. Gomez***

8:25 Paper 266b: Lignocellulosic Biomass Pretreatment Using Radical Species — ***Maryam Davaritouchaee****, Shulin Chen*

8:50 Paper 266c: Stabilization of Carbohydrates with Formaldehyde During Integrated Biomass Depolymerization
— ***Ydna M. Questell-Santiago****, Masoud Talebi Amiri, Li Shuai, Jeremy S. Luterbacher*

9:15 Paper 266d: Milling, Crystallinity and Pyrolysis Rates for Cellulose and Whole Biomass — *Matthew Kelley, Abdul Salam Mohammad, Ali Zolghadr,* ***Joseph Biernacki****, Scott Northrup*

9:40 Paper 266e: Effect of Pretreatment on Biomass Pyrolysis for Better Quality of Bio-Oil — ***Yuan Xue****, Joel Braden, Xianglan Bai*

10:05 Paper 266f: An Examination of Ash from Fast Pyrolysis
— ***Dane Erickson****, Theodore J. Heindel*

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(267) Biomaterial Scaffolds for Tissue Engineering I: Anisotropic Materials
Tuesday, Oct 31, 8:00 AM
MCC, 209A/B

Cole DeForest, Chair
Yan Li, Co-Chair

Sponsored by: Biomaterials

8:00 Paper 267a: Multiplicity of Morphologies in Poly (L-lactide) Bioresorbable Vascular Scaffolds — *Artemis Ailianou, Karthik Ramachandran, Mary Beth Kossuth, James Paul Oberhauser,* ***Julia A. Kornfield***

8:18 Paper 267b: Tissue Response and Integration in Biomaterial Implants Derived from Morphologically Unique Emulsion Gels — ***Todd Thorson****, Ali Mohraz, Elliot Botvinick*

8:36 Paper 267c: Surface Tension-Assisted Additive Manufacturing of Multicomponent Biomaterials
— ***Mark W. Tibbitt****, Héloïse Ragelle, Michael Cima, Robert Langer*

8:54 Paper 267d: Development of Gelatin- and Graphene-Based Conduits Using 3D Printing Strategies for the Transdifferentiation of Mesenchymal Stem Cells into Schwann Cell-Like Phenotypes Through Electrical Stimuli
— ***Metin Uz****, Maxsam Donta, Donald S. Sakaguchi, Surya K. Mallapragada*

9:12 Paper 267e: Effect of Molecular Weight and Degree of Functionality on Degradation, Biocompatibility and Two-Photon Polymerization of Acrylated Poly(caprolactone)
— ***Brian J. Green****, Jessica Thompson, Kristan S. Worthington, Budd A. Tucker, C. Allan Guymon*

9:30 Paper 267f: An Injectable and Anisotropic Hydrogel with Biomimetic Structures for Directed Cell and Nerve Growth — ***Jonas C. Rose****, David B. Gehlen, Esther Jaekel, Jens Köhler, Khosrow Rahimi, Martin Möller, Laura De Laporte*

9:48 Paper 267g: Engineering Extracellular Matrix Mimetic Materials by Green Electrospinning of Collagen
— ***Jorge Almodovar****, David Castilla*

10:06 Paper 267h: Biomimetic Scaffolds for In-Vitro Bone Marrow Tissue Engineering — *Yongkuk Park, Ryan Carpenter,* ***Jungwoo Lee***

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(268) Bionanotechnology Graduate Student Award Session
Tuesday, Oct 31, 8:00 AM
MCC, 212A/B

Samantha A. Meenach, Chair
Kathryn A. Whitehead, Co-Chair
Millicent Sullivan, Co-Chair

Sponsored by: Bionanotechnology

8:00 Paper 268a: Award Submission: Laser-Activated Tissue-Integrating Sutures for Rapid Closure of Soft Tissue Wounds — ***Russell Urie****, Deepanjan Ghosh, Tanner Flake, Jerry Crum, Jacquelyn Kilbourne, Kaushal Rege*

8:20 Paper 268b: Award Submission: Construction of Biomimetic Photocathodes Using Photosystem I-Proteoliposomes Supported on Substrates — ***Hanieh Niroomand****, Ravi Pamu, Dibyendu Mukherjee, Bamin Khomami*

8:40 Paper 268c: Award Submission: Carbon Nanotube-Assisted Delivery of Genetic Material into Mature Plants
— ***Gozde Sultan Demirer****, Markita Landry*

9:00 Paper 268d: Award Submission: Engineering Surface-Functionalized, Intelligent Hydrogel Nanoparticles with Tunable Release Properties
— ***Angela Wagner****, Noor Al-Sayyad, Alexandria Lawrence, Nicholas A. Peppas*

9:20 Paper 268e: Award Submission: Tumor-Penetrating Aerosol Nanocomposite Microparticles for the Treatment of Lung Cancer
— ***Elisa A. Torrico-Guzmán****, Samantha A. Meenach*

9:40 Paper 268f: Award Submission: Oral Delivery of siRNA Lipid Nanoparticles: Fate in the GI Tract
— ***Rebecca Ball****, Palak Bajaj, Kathryn A. Whitehead*

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(269) Catalysis with Microporous and Mesoporous Materials I
Tuesday, Oct 31, 8:00 AM
MCC, L100A

Michele Sarazen, Chair
Dongxia Liu, Co-Chair
Marat Orazov, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

8:00 Paper 269a: Introducing Catalytic Diversity into Single-Site Zeolites of Fixed Composition via Synthetic Control of Active Site Proximity
— ***John R. Di Iorio****, Claire T. Nimlos, Rajamani Gounder*

8:18 Paper 269b: Probing the Site-Pairing Preference of Framework Aluminum in ZSM-5 with $Ga(CH_3)_3$
— ***Kyle Groden****, Zachary Jones, Renqin Zhang, Susannah L. Scott, Jean-Sabin McEwen*

8:36 Paper 269c: Quantitative Analysis of Catalysis in Hierarchical Zeolites and Surface Topology Effect Based on MFI and MWW Frameworks — ***Dandan Xu****, Sang Hyun Ahn, Limin Ren, Anatoliy Kuznetsov, Dongxia Liu, Suk Bong Hong, Michael Tsapatsis*

8:54 Paper 269d: Multi-Faceted Approach to Optimize ZSM-11 Catalysts for Methanol-to-Hydrocarbon Reactions — ***Yufeng Shen****, Thuy T. Le, Jeffrey D. Rimer*

9:12 Paper 269e: Atomic-Level Insights into Molecular Adsorption and Reaction Properties at Distinct Heteroatom Sites in Aluminosilicate Zeolite Catalysts — ***Zachariah Berkson****, Subramanian Prasad, Bradley F. Chmelka*

9:30 Paper 269f: Synthesis and SCR Testing of SSZ-39 — ***Daniel Shantz****, Ross Ransom, Jonathan Coote, Roger Moulton, Feng Gao*

9:48 Paper 269g: Determining Siting Preference of Exchanged Fe Ions in Fe-SSZ-13 Zeolite Through Density Functional Theory and Ab-Initio Molecular Dynamics — ***Sichi Ll****, William F. Schneider*

10:06 Paper 269h: Fabrication of Bifunctional Acid-Base Catalyst by Organic Pillared MFI Nanosheets
— ***Baoyu Liu***

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(270) Catalytic Processing of Fossil and Biorenewable Feedstocks IV: Chemistry of Furanics
Tuesday, Oct 31, 8:00 AM
MCC, L100C

Ning Yan, Chair
George Tsilomelekis, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

8:00 Paper 270a: Production of Furandicarboxylic Acid (FDCA) Using Biomass-Derived γ-Valerolactone
— ***Ali Hussain Motagamwala****, David Martin Alonso, Wangyun Won, Christos T. Maravelias, James A. Dumesic*

8:20 Paper 270b: Spectroscopic and Modeling Study of Aluminum Active Species in Glucose Isomerization
— ***Angela Norton****, Hannah Nguyen, Dionisios G. Vlachos*

8:40 Paper 270c: Hydrodeoxygenation of Furfural over Multifunctional Catalysts — ***Konstantinos A. Goulas****, Alexander V. Mironenko, Glen R. Jenness, Vassili Vorotnikov, Tobias Mazal, Dionisios G. Vlachos*

9:00 Paper 270d: Functionalization of 5-Hydroxymethylfurfural by Selective Etherification — *Meredith Allen, William M. Gramlich,* ***Thomas J. Schwartz***

9:20 Paper 270e: Inhibition of Xylene Isomerization in the Production of Renewable Aromatic Chemicals from Biomass-Derived Furans
— ***Katherine P. Vinter****, C. Luke Williams, Ryan Patet, Chun-Chih Chang, Nima Nikbin, Shuting Feng, Matthew R. Wiatrowski, Stavros Caratzoulas, Wei Fan, Dionisios G. Vlachos, Paul J. Dauenhauer*

9:40 Paper 270f: Renewable Butadiene Production from Tetrahydrofuran over HZSM-5 — ***Sha Li****, Omar A. Abdelrahman, Paul J. Dauenhauer, Dionisios G. Vlachos, Stavros Caratzoulas*

10:00 Paper 270g: Reaction Mechanisms Responsible for the Selective Vapor-Phase Rearrangement of Furanics — *Valeria Herrera, Nicholas M. Briggs, Bin Wang,* ***Steven Crossley***

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(271) Cell Adhesion and Migration I
Tuesday, Oct 31, 8:00 AM
MCC, 208B

Matthew Paszek, Chair
Carla M. R. Lacerda, Co-Chair
Nitin Agrawal, Co-Chair

Sponsored by:
Engineering Fundamentals in Life Science

8:00 Paper 271a: Focal Adhesion Architecture and Composition Regulate Cell Adhesion and Traction Generation Independent of Integrin Class
— ***Steven J. Tan****, Alice C. Chang, Cayla M. Miller, Alexander R. Dunn*

8:18 Paper 271b: Cells Migration on Micropatterns Through the Epithelial-Mesenchymal Transition
— ***Tzu Chieh Chao***

8:36 Paper 271c: Quantifying Tissue-Induced Collagen Fiber Alignment in 3D Microfabricated Tissues
— ***Bryan A. Nerger****, Alexandra Piotrowski-Daspit, Abraham Wolf, Sankaran Sundaresan, Celeste M. Nelson*

8:54 Paper 271d: Evaluation of Preliminary Adhesion Processes of Cyanobacteria (Blue-Green Algae) on Photobioreactor Materials
— ***Suvarna N. L. Talluri****, Robb M. Winter, David R. Salem*

9:12 Paper 271e: CDC42 Regulates Formation of Branches During Chemotactic Invasion of 3D Angiogenic Sprouting — ***Duc-Huy Nguyen****, Lin Gao, Alec Wong, Christopher Chen*

9:30 Paper 271f: Solid Surface Tension of Biomaterials Direct Cellular Behaviors Through Integrins
— ***Zhu Cheng****, Carolyn Shurer, Chung-Yuen Hui, Matthew Paszek*

9:48 Paper 271g: Migration Against the Direction of Flow Is LFA-1 Dependent in Human Hematopoietic Stem and Progenitor Cells
— ***Alexander Buffone Jr.****, Nicholas Anderson, Daniel A. Hammer*

10:06 Paper 271h: Patterned Cell Alignment in Response to Macroscale Curvature and Rho Activation
— ***Nathan D. Bade****, Randall D. Kamien, Richard K. Assoian, Kathleen J. Stebe*

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(272) Charged Polymers for Membrane-Based Water and Energy Applications
Tuesday, Oct 31, 8:00 AM
MCC, M100I

Geoffrey M. Geise, Chair
William Phillip, Co-Chair
Ayse Asatekin, Co-Chair

Sponsored by: Polymers

8:00 Paper 272a: Recent Advancements in Reactive Electrochemical Membrane Development for Water Treatment
— ***Brian Chaplin****, Yin Jing, Pralay Gayen, Sasmita Nayak*

8:20 Paper 272b: Rational Design of Ion-Exchange Membranes for Low-Energy Brackish Water Desalination via Membrane Capacitive Deionization — ***Christopher G. Arges****, Varada Menon Palakkal*

8:40 Paper 272c: Inkjet Printing of Charge Mosaic Membranes as a Method for Tailored Aqueous Separation — ***Mark J. Summe****, William A. Phillip*

9:00 Paper 272d: Ion-Specific Effects in Charged Polymer Membranes for Water Purification — ***Geoffrey M. Geise***

9:20 Paper 272e: 3D Morphological Characterization of the Polyamide Active Layer of Reverse-Osmosis Membranes Using TEM and Soft X-Ray Scattering — *Tyler Culp,* ***Yuexiao Shen****, Mou Paul, Abhishek Roy, Steve Rosenberg, Michael Behr, Cheng Wang, Manish Kumar, Enrique D. Gomez*

9:40 Paper 272f: Thermodynamic Modeling of Ion-Exchange Membranes with eNRTL Model — ***Yue Yu****, Ni Yan, Michele Galizia, Benny D. Freeman, Chau-Chyun Chen*

10:00 Paper 272g: Ion Partitioning Between Brines and Ion-Exchange Polymers — ***Michele Galizia****, Donald R. Paul, Benny D. Freeman*

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(273) Combustion Kinetics and Emissions I
Tuesday, Oct 31, 8:00 AM
MCC, L100F

Bihter Padak, Chair
Erdem Sasmaz, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

8:00 Paper 273a: Implications of High-Accuracy Thermochemical Kinetics for $H + CH_3$ (+M) ⇄ CH_4 (+M) on Combustion Models
— ***Nicole Labbe****, Ahren Jasper, Raghu Sivaramakrishnan, Stephen J. Klippenstein, James A. Miller, Branko Ruscic*

8:22 Paper 273b: Estimation of Thermodynamic Properties of Polycyclic Molecules by a Linear Regression Model — ***Yi-Pei Li***, *Kehang Han, William H. Green*

8:44 Paper 273c: Hydrogen Binding Versus Dissociation During Soot Formation: Insights from Reactive Molecular Dynamics — ***Eirini Goudeli***, *Christopher J. Hogan Jr.*

9:06 Paper 273d: Effect of Composition Variation of Syngas Mixtures on NO_x Formation at High Pressure — ***Nazli Asgari***, *Bihter Padak*

9:28 Paper 273e: Numerical Modelling of Industrial Burners for Reduction of NO_x Emissions Using Flamelet Methods in Combination with a Newly Developed Postprocessor for Fast and Accurate Emission Prediction — ***Werner Rudolf Pollhammer,*** *Christoph Spijker, Harald Raupenstrauch, Michael Koller*

9:50 Paper 273f: A CFD Model-Based Optimization of a Low-NO_x Burner in Integrated Process System — ***Mohsen Behnam***, *Paul Gaffuri, Jordan Mcginty, Zhijiang Li*

10:12 Paper 273g: Mapping the Stable Region of Operation of Homogenously Charged Compression Ignition (HCCI) Engine for Methane and DMF Fuel Blend — ***Gokul Venugopalan***, ***Pratheeba Chanda Nagarajan***, *Arunagiri P.*

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(274) Continuous Processing Technologies Applied in Drug Product Development

Tuesday, Oct 31, 8:00 AM
MCC, 204A/B

Joe Hannon, Chair
Mark Barrett, Co-Chair

Sponsored by:
Pharmaceutical Discovery, Development and Manufacturing Forum

8:00 Paper 274a: How Raw Material Attributes and Process Parameters Affect the Global Residence Time Distribution Behavior in Continuous Direct Compression — ***Samantha Hurley***, *Robert F. Meyer, Brendon G. Ricart, Matthew H. Flamm, Frank D. Witulski*

8:22 Paper 274b: Development of a Continuous Blending System — ***Daniel Borginis***

8:44 Paper 274c: Investigating Continuous Powder Blending at Different Scales Using Residence Time Distribution Studies — ***Marcus O'Mahony***, *Steven Dale, Greg Connelly, Joseph W. Bullard, Pongpumin Bunchatheeravate*

9:06 Paper 274d: Leveraging Raw Material and Blend Properties with the Die-Filling Step of the Tableting Process — ***Valérie Vanhoorne,*** *Bernd Van Snick, Jens Dhondt, Celine Segers, Kato Van Vooren, Thomas Eerdekens, Giustino Di Pretoro, Thomas De Beer, Chris Vervaet*

9:28 Paper 274e: Modelling of Pharmaceutical HME Processes — ***Josip Matić***, *Milica Stanković-Brandl, Amrit Paudel, Johannes G. Khinast, Christophe Herkenne, Jessica Lovey Martinetti, Sophie Martel*

9:50 Paper 274f: In-Depth Experimental Analysis of Pharmaceutical Twin-Screw Wet Granulation in View of Detailed Process Understanding — ***Maxim Verstraeten,*** *Daan Van Hauwermeiren, Kai Lee, Neil Turnbull, Pankaj Doshi, Mary T. am Ende, Ingmar Nopens, Thomas De Beer*

10:12 Paper 274g: Understanding the Impact of Feed Frame Design and Process Parameters on the Die-Filling Step of the Tableting Process — ***Wouter Grymonpré***, *Valérie Vanhoorne, Bernd Van Snick, Thomas De Beer, Jean Paul Remon, Chris Vervaet*

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(275) Conversion of Solid Wastes to Energy and/or Product

Tuesday, Oct 31, 8:00 AM
MCC, 103B

Zheng Liu, Chair
Hsi-Wu Wong, Co-Chair
Sudhagar Mani, Co-Chair

Sponsored by:
Innovations of Green Process Engineering for Sustainable Energy and Environment

8:00 Paper 275a: Economic Assessment and Scale-Up of an Eco-Friendly Continuous Bioleaching System for Recovery of Rare Earth Elements from End-of-Life Materials — ***David W. Reed***, *Vicki S. Thompson, Mayank Gupta, Honqyue Jin, Michael Jindra, Van Nguyen, Yoshiko Fujita, John Sutherland, Yongqin Jiao*

8:18 Paper 275b: One-Pot Production of Furans from Industrial Hemp — ***Md. Anwar Hossain***, *Thanh Khoa Phung, Sarttrawut Tulaphol, Teerawit Prasomsri, Noppadon Sathitsuksanoh*

8:36 Paper 275c: Catalytic Depolymerization of Lignin over Mesoporous Solid Lewis Acid Catalysts — ***Kakasaheb Nandiwale***, *Andrew Danby, Anand Ramanathan, Raghunath V. Chaudhari, Bala Subramaniam*

8:54 Break

9:12 Paper 275e: Sustainable Energy Production from Renewable Resources Through Anaerobic Digestion Process: Nigerian Experience — ***Oluyemi Adetule***

9:30 Paper 275f: Fractionation of Tyre Pyrolysis Oil for Generation of Value-Added Products — *Ruturaj Sawant,* ***Abhishek Sharma***, *Jyeshtharaj B. Joshi*

9:48 Paper 275g: Catalytic Conversion of Biomass-Derived Lactones into Fuels and Chemicals — *Md. Imteyaz Alam, Shelaka Gupta, Ashish Bohre, Ejaz Ahmad, Tuhin Suvra Khan, Basudeb Saha,* ***M. Ali Haider***

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(276) CO_2 Capture by Adsorption I: Process and Storage

Tuesday, Oct 31, 8:00 AM
MCC, M100F

Jian Liu, Chair
Joshua Thompson, Co-Chair

Sponsored by:
Adsorption and Ion Exchange

8:00 Paper 276a: Multiscale Screening of Porous Materials for Carbon Capture — ***Shreenath Krishnamurthy***, *Amir H. Farmahini, Richard J. Gowers, Daniel Friedrich, Maria-Chiara Ferrari, Stefano Brandani, Lev Sarkisov*

8:22 Paper 276b: Evaluation of Diamine-Appended Metal-Organic Frameworks for Post-Combustion CO_2 Capture Using a VPSA — ***Kasturi N. Pai***, *Joha Baboolal, Dave Sharp, Arvind Rajendran*

8:44 Paper 276c: Sub-Ambient Pressure Swing Adsorption for Enhanced Post-Combustion Carbon Dioxide Capture via Phase-Change Materials Application — ***Héctor Octavio Rubiera Landa***, *Stephen J. A. DeWitt, Matthew J. Realff, Ryan P. Lively, Yoshiaki Kawajiri*

9:06 Paper 276d: Atmospheric CO_2 Capture via Temperature/Vacuum Swing Adsorption in SIFSIX-3-Ni — ***Eleni Tsalaporta***, *Sebastien Vaesen, Guanghua Jin, J. M. D. Macelroy, Wolfgang Schmitt*

9:28 Paper 276e: Pressure Swing Adsorption Cycle Synthesis Utilizing Artificial Neural Networks as Surrogate Models — ***Karson Leperi***, *Fengqi You, Randall Q. Snurr*

9:50 Paper 276f: Process Flowsheet Optimization and Techno-Economic Assessment of Post-Combustion CO_2 Capture Using Heat-Integrated, Sub-Ambient PSA — ***Rohan Awati***, *David Sholl, Ryan Lively, Yoshiaki Kawajiri, Matthew Realff, Héctor Octavio Rubiera Landa, Stephen J. A. DeWitt*

10:12 Paper 276g: Fast Sorbent–Mediated Water-Gas Shift (C-SHIFT) Process for Pre-Combustion CO_2 Capture — ***Johannis A. Z. Pieterse***, *Matthew E. Boot-Handford, Paul S. Fennell, Paul D. Cobden, Jurriaan Boon, Mark G. Sceats, Brain N. C. Sweeney, Bjornar Arstad, Richard Blom*

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(277) Crystallization Process Development

Tuesday, Oct 31, 8:00 AM
MCC, 102B

James C. Marek, Chair
Tom Xu, Co-Chair

Sponsored by:
Process Research and Innovation

8:00 Paper 277a: Chiral Control of Enantiomers Through Crystallization: Moving from Ternary Phase Diagrams to Design Spaces — ***Michael Lovette***

8:20 Paper 277b: Leveraging Mechanistic Understanding of Impurity Rejection During Crystallization for Rational Process Design — ***Eric Sirota***

8:40 Paper 277c: Development of Combined Continuous Reaction to Crystallization Process Using PAT Tools — ***Gladys Kate Pascual***, *Roderick Jones, Philip Donnellan, Brian Glennon*

9:00 Paper 277d: Process Design to Preserve Particle Properties During Crystallization of Energetic Material — ***Sarah Rothstein***, *Jerry S. Salan, Matthew Jorgensen, Jamie Corwel, Sarah Keshishian*

9:20 Paper 277e: Multiscale and Multi-Purpose Modelling for In-Silico Designing and Optimization of Pharmaceutical Crystallization Process — ***Getachew S. Molla***, *Merve Öner, Jens Abildskov, Gürkan Sin*

9:40 Paper 277f: Sensitivity Analysis and Optimization Study of Pharmaceutical Crystallization Process — ***Merve Öner***, *Getachew S. Molla, Michael Frederick Freitag, Stuart Michael Stocks, Jens Abildskov, Gürkan Sin*

10:00 Paper 277g: Segmented Continuous Crystallization Process Optimization — ***Min Su***, *Yanyan Gao*

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(278) Design, Construction and Operation of Unit Operations Labs and Pilot Plants

Tuesday, Oct 31, 8:00 AM
MCC, 102C

Michael Trainor, Chair
Vinod Kumar Venkatakrishnan, Co-Chair

Sponsored by: Pilot Plants

8:00 Paper 278a: Biochar Collection Overview and Design Upgrades in Biomass Pyrolysis Pilot Plant — ***Tim Dunning***, *Esther Wilcox*

8:25 Paper 278b: Advances of Syngas Chemical-Looping Process at the Ohio State University: Pilot Demonstration and Advanced Control Architecture Development — ***Tien-Lin Hsieh,*** *Dikai Xu, Sourabh Nadgouda, Cheng Chung, Yitao Zhang, Yaswanth Pottimurthy, Mengqing Guo, Yu-Yen Chen, Mingyuan Xu, Cody Park, Dawei Wang, Liang-Shih Fan,* ***Andrew Tong***

8:50 Paper 278c: Design of a Continuous Laboratory Setup — ***Ruth Morais***, *Filipe Ataíde, Nuno Matos, Luis Olival*

9:15 Paper 278d: A Novel Process for Continuous Magnesium Metal Production by Carbothermal Reduction of Magnesium Oxide — ***Boris Chubukov***, *Aaron W. Palumbo, Scott Rowe, Mark Wallace, Alan W. Weimer*

9:40 Break

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(279) Developments in Petroleum and Biofuels Refining Technologies I

Tuesday, Oct 31, 8:00 AM
MCC, 200A

Ronald Hedden, Chair
Ian M. Glasgow, Co-Chair
Umakanta Jena, Co-Chair

Sponsored by:
Fuels and Petrochemicals Division

8:00 Paper 279a: Modifying a Davison Circulating Riser to Accommodate Biomass-Derived Feedstocks — ***Jessica Olstad***, *Mark Jarvis, Yves Parent, Kim Magrini*

8:25 Paper 279b: Numerical Evaluation of a Fluid Catalytic Cracking Unit with Internal Baffles — *Tania Sanchez Martinez, Leonardo M. Rosa,* ***Jonathan Utzig***, *Waldir Pedro Martignoni, Henry F. Meier*

8:50 Paper 279c: Technical Method for Reducing the Coking Rate of the Refinery Furnace — ***Junwei Yang***

9:15 Paper 279d: A Group Contribution Method for the Prediction of the Mid-Infrared (MIR) Absorption Spectra of Species Involved in Fluid Catalytic Cracking (FCC) — ***Sandra Milena Lopez-Zamora***, *Hugo de Lasa, Alejandro Molina*

9:40 Break

10:05 Paper 279f: A Method of Directional Separation of Key Component in FCC Gasoline to Reduce Commercial Gasoline Octane Number Loss — ***Yuhao Zhang***, *Liang Zhao, Jinsen Gao, Chunming Xu*

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(280) Diversity and Inclusion: Starting and Thriving in the Workplace (Invited Talks)

Tuesday, Oct 31, 11:00 AM
MCC, 101G

Adrienne Minerick, Co-Chair
Kathy Lee, Co-Chair
Helen Buettner, Co-Chair
Dwayne Mays, Co-Chair

Sponsored by:
Undergraduate Education

11:00 Introductory Remarks

11:10 Paper 280d: Re-situating the Professional Formation of Engineers at Oregon State University — ***Jim Sweeney***

11:25 Paper 280a: Chevron — ***Cynthia Murphy***, *S. Shariq Yosufzai*

11:40 Paper 280b: BASF — ***Mike McAtee***

11:55 Paper 280c: ExxonMobil's Diversity and Inclusion Efforts – Creating a Premier Global Workforce that Works to Help Power the World's Progress — ***Yuk Louie***

12:10 Panel Discussion — ***Zenaida Gephardt***

12:55 Concluding Remarks

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(281) Dynamics and Modeling of Particles, Crystals and Agglomerate Formation

Tuesday, Oct 31, 8:00 AM
MCC, 200H

Tao Wei, Chair
Priscilla J. Hill, Co-Chair

Sponsored by:
Particle Production and Characterization

8:00 Paper 281a: Dynamics of Protein Aggregation: Crowding Effect in Confined Environment — ***Size Zheng***, *Katherine S. Shing, Muhammad Sahimi*

8:22 Paper 281b: Modified-Laguerre Polynomials for Distribution Reconstruction from Moments — ***R. Bertrum Diemer Jr.***

8:44 Paper 281c: Solution Space Mapping for Power-Law Aggregation Rate Kernels — ***R. Bertrum Diemer Jr.***

9:06 Paper 281d: Nucleation and Agglomeration of Hydrate Particles in Gas-Liquid Multiphase Flow Systems — ***Lin Ding***, *Bohui Shi, Yang Liu, Shangfei Song, Jing Gong*

9:28 Paper 281e: Simplifying the Population Balance for Teaching Kinetics & Contactor Design in Particle Processing — ***R. Bertrum Diemer Jr.***

9:50 Paper 281f: Mapping the General 1-D Population Balance Solution Space — ***R. Bertrum Diemer Jr.***

10:12 Paper 281g: Noble Method for Evaluating the Distributive Mixing of Bimodal Lagrangian Particles — ***Chanho Park***, *Jiheon Lee, Hyungtae Cho, Youngjin Kim, Il Moon*

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(282) Electrocatalysis and Photoelectrocatalysis IV: ORR/OER

Tuesday, Oct 31, 8:00 AM
MCC, L100D

Zhenmeng Peng, Chair
Timothy Van Cleve, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

8:00 Paper 282a: Rational Design and Synthesis of Surfactant-Free Pt-Based Ternary Nanoalloys as Superior Oxygen Reduction Reaction Electrocatalysts — ***Sheng Hu***, *Bamin Khomami, Dibyendu Mukherjee*

8:18 Paper 282b: Low-Platinum Electrocatalysts for the Oxygen Reduction Reaction at Fuel Cell Cathodes — ***Maha Yusuf***

8:36 Paper 282c: Improved Activity and Durability of Ionic Liquid Composite Nanoporous Nanoparticle Electrocatalysts for Oxygen Reduction Reaction — ***Yawei Li***, *Joshua Snyder*

8:54 Paper 282d: Particle Atomic Layer Deposition for Stabilization of Oxygen Reduction Catalysts — ***William McNeary IV,*** *Audrey Linico, Megan Maguire, Alia M. Lubers, Alan W. Weimer*

9:12 Paper 282e: A Mechanistic Insight into the Electrocatalytic Behavior of Mixed Oxide Cathode Catalysts for Li-O_2 Batteries — ***Samji Samira***, *Ayad Nacy, Eranda Nikolla*

9:30 Paper 282f: Characterization of FeNi-Alloy Nanoparticles for OER as a Function of Iron-Nickel Composition — *Prashant Acharya, Zachary Nelson,* ***Lauren F. Greenlee***

9:48 Paper 282g: Active Sites in Nitrogen-Doped Carbon Nanostructures for Oxygen Reduction and Oxygen Evolution Reactions — *Kuldeep Mamtani,* ***Deeksha Jain***, *Anne Co, Umit S. Ozkan*

10:06 Paper 282h: Atomic Iron-Dispersed Electrocatalysts Derived from Metal-Organic Framework for Oxygen Reduction — *Hanguang Zhang,* ***Gang Wu***

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(283) Energy Sustainability: Challenges and Solutions

Tuesday, Oct 31, 8:00 AM
MCC, 101H

William M. Barrett, Chair
Emre Gençer, Co-Chair
Vikas Khanna, Co-Chair

Sponsored by: Sustainable Energy

8:00 Paper 283a: A General Data-Driven Method for Analysis of Energy Efficiency in Manufacturing Zones — ***Aida Amini Rankouhi***, *Yinlun Huang*

8:19 Paper 283b: Optimal Design of Multi-Enterprise Industrial Waste-to-Energy Networks Under Uncertain Conditions — ***Vasco Bolis***, *Elisabet Capón-García, Konrad Hungerbuehler*

8:38 Paper 283c: Survey-Driven Sustainability Assessment Using Global Optimization Techniques — ***Jeremy A. Conner***, *Vasilios Manousiouthakis*

8:57 Paper 283d: On the Likely Competition for Land Between Food and Energy in a Solar Economy — ***Caleb Miskin***, *Yiru Li, Rakesh Agrawal*

9:16 Paper 283e: Energy-Efficient Design of Ionic Liquid–Based Gas Separation Processes — ***Xinyan Liu***, *Xiaodong Liang, Rafiqul Gani, Xiangping Zhang, Suojiang Zhang*

9:35 Paper 283f: Maximising the Mitigation Potential of Curtailed Wind: A Comparison Between Carbon Capture and Utilisation, and Direct Air Capture Processes for the UK — ***Habiba A. Daggash***, *Clemens Patzschke, Clara F. Heuberger, Lingqiao Zhu, Niall Mac Dowell*

9:54 Paper 283g: Thermodynamic Model-Based Synthesis Methodology to Design Optimal Heat-Integrated Work Exchanger Network — ***Aida Amini Rankouhi***, *Yinlun Huang*

10:13 Paper 283h: Optimal Use of LNG Cold Energy in Air Separation Units
*— **Donghoi Kim**, Roxane Giametta, Truls Gundersen*

(284) Estimation and Control of Uncertain Systems
Tuesday, Oct 31, 8:00 AM
MCC, 103D

Ali Mesbah, Chair
Joseph Scott, Co-Chair

Sponsored by:
Systems and Process Control

8:00 Paper 284a: Model-Based Approach to the Online Identification of the Optimal Uncertainty Set Within Stochastic Dynamic Optimization & Optimal Control Algorithms
*— **Francesco Rossi,** Flavio Manenti, Guido Buzzi-Ferraris, Gintaras Reklaitis*

8:19 Paper 284b: Autocovariance-Based Model Mismatch Diagnosis for MPC with State Estimation
*— **Jodie Simkoff**, Siyun Wang, Michael Baldea, Leo H. Chiang, Ivan Castillo, Rahul Bindlish, David Stanley*

8:38 Paper 284c: A Tractable Method for Closed-Loop Active Fault Diagnosis of Stochastic Linear Systems
*— **Tor Aksel N. Heirung**, Joel Paulson, Richard D. Braatz, Ali Mesbah*

8:57 Paper 284d: Set-Membership Nonlinear Regression Approach to Parameter Estimation *— Nikola D. Peric, **Benoit Chachuat***

9:16 Paper 284e: Model Predictive Control Under Model Structural Uncertainty *— **Dinesh Krishnamoorthy**, Bjarne Foss, Sigurd Skogestad*

9:35 Paper 284f: Passivity-Based Observer and Application in Reaction Heat Estimation *— **Zixi Zhao**, B. Erik Ydstie*

9:54 Paper 284g: Parameter Estimation and Process Optimization of Heterogeneous Batch Reactors Under Uncertainty *— **Yajun Wang**, Mukund Patel, John Wassick, Lorenz Biegler*

10:13 Paper 284h: Rapid and Accurate Fault Detection and Diagnosis for Uncertain Nonlinear Systems Using Advanced Set-Based State Estimation Techniques *— Xuejiao Yang, Kai Shen, **Joseph Scott***

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(285) Fluid-Particle Flow and Reaction Systems I — In Honor of Professor L. S. Fan
Tuesday, Oct 31, 8:00 AM
MCC, 200I

Robert Pfeffer, Chair
Fanxing Li, Co-Chair

Sponsored by:
Fluidization and Fluid-Particle Systems

8:00 Introductory Remarks
*— **R. Pfeffer***

8:10 Paper 285a: Cyclone Dipleg Design and Operation Considerations
*— **Ted Knowlton***

8:35 Paper 285b: Effect of Particle-Wall Interactions in Freeboard of Gas-Solid Fluidized Beds on Tribo-Electrification and Entrainment of Fines
*— Farzam Fotovat, **John R. Grace**, **Xiaotao Bi***

9:00 Paper 285c: Innovative Cyclone Technology: A Common Denominator for Many Successful Fluidization Processes *— **Ye-Mon Chen**, Ted Knowlton, S. B. Reddy Karri*

9:25 Paper 285d: A Fluidized-Bed "Thermochemical Battery" for Concentrated Solar Power Applications
*— Claudio Tregambi, Fabio Montagnaro, **Piero Salatino**, Roberto Solimene*

9:50 Paper 285e: An Innovative Hydrogen and Power Coproduction System Using Integrated Exergy Recuperative Biomass Gasification and SOFC *— **Atsushi Tsutsumi**, Masanori Ishizuka, Kaduo Tsutsumi, Tomohiro Ishizuka*

10:15 Paper 285f: Flow Structures in Circulating Fluidized-Bed Risers: From Dilute to High-Density Gas-Solid Flow
*— **Timo Hensler**, Karl-Ernst Wirth*

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(286) Gas Hydrates Science and Engineering
Tuesday, Oct 31, 8:00 AM
MCC, L100I

Amadeu K. Sum, Chair

Sponsored by:
Thermodynamics and Transport Properties

8:00 Paper 286a: Nucleation Mechanism of Clathrate Hydrates of Soluble Guest Molecules
*— **Ryan DeFever**, Sapna Sarupria*

8:17 Paper 286b: Investigation on Thermophysical Properties of Structure II Clathrate Hydrates Using Molecular Dynamics Simulations *— Bing Fang, **Fulong Ning**, Ping Cao, Jianyang Wu, Thijs J. H. Vlugt, Signe Kjelstrup*

8:34 Paper 286c: Prediction of Gas Hydrate Formation Conditions in Brine Systems with the eNRTL Model
*— **Amadeu K. Sum**, Yue Hu*

8:51 Paper 286d: Clathrate Hydrate Formation Using Fluorocarbons
*— **M. Alejandra Rocha**, Mark B. Shiflett*

9:08 Paper 286e: Methane Hydrate Formation Accelerated with Various Promoters in an Unstirred Reactor
*— Seungjun Baek, Yun-Ho Ahn, Junshe Zhang, Juwon Min, Huen Lee, **Jae W. Lee***

9:25 Paper 286f: Effect of Thermodynamic Promoter (TBAB) in Gas Hydrates Dissociation Conditions of the Mixture $H_2O + CO_2$ + Undecane
*— Raúl A. Santos-Serena, Pedro Esquivel-Mora, Jose J. Castro-Arellano, **Luis A. Galicia-Luna***

9:42 Paper 286g: Study on Flow Behavior of CO_2-in-Water (C/W) Emulsion in the Porous Medium Under Hydrate Stability Conditions
*— **Yoshihiro Masuda**, Keishi Usui, Yuta Tosuji, Shigemi Naganawa, Masahiro Yasue, Yunfeng Liang, Norio Tenma*

9:59 Paper 286h: Ionic Liquids as Dual Functional Inhibitors for Natural Gas Hydrates *— **Majeda Khraisheh Sr.***

10:16 Paper 286i: Modeling of Gas Hydrate Equilibria for CO_2-N_2-Water System by SAFT Approach *— **Arsalan Hejrati**, **Chongwei Xiao***

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(287) Graphene 2-D Materials: Synthesis, Functions and Applications I
Tuesday, Oct 31, 8:00 AM
MCC, 213A/B

Lei Li, Chair
Dorsa Parviz, Co-Chair
Ryan M. Paul, Co-Chair

Sponsored by: Carbon Nanomaterials

8:00 Paper 287a: Invited: Chemical, Interfacial, and Opto/Electronic Properties of CVD-Grown Graphene, hBN, MoS_2, WS_2 and Their Heterostructures *— **Vikas Berry***

8:30 Paper 287b: Development of Accurate Potentials to Explore the Structure of Water on 2-D Materials
*— Karteek K. Bejagam, Samrendra Singh, **Sanket A. Deshmukh***

8:50 Paper 287c: Fabrication of High-Quality Graphene Nanobelts for Supercapacitor *— Tianju Fan, Tingting He, Yidong Liu, **Yong Min***

9:10 Paper 287d: Ionophore-Decorated Phosphazene-Functionalized Magnetic Graphene Oxide as a Composite Adsorbent Material for Selective Lithium Ion Recovery *— **Khino J. Parohinog**, Grace M. Nisola, Wook-Jin Chung*

9:30 Paper 287e: Evaluation of Sulfur Role as a Promoter for the Growth of Carbon Nanotube in Chemical Vapor Deposition *— **Shunsuke Suzuki**, Shinsuke Mori*

9:50 Paper 287f: Direct Growth of Unstacked Double-Layer Graphene and Graphene/Single-Walled Carbon Nanotube Hybrids for Li-S Batteries
*— **Mengqiang Zhao**, Qiang Zhang, Fei Wei*

10:10 Paper 557e: Hybrid Carbon Nanostructures for Electrochemical Energy Storage*— **Min Kyu Song***

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(288) Highly Selective Separations with Membranes
Tuesday, Oct 31, 8:00 AM
MCC, M100D

Dibakar Bhattacharyya, Chair
Stephen Ritchie, Co-Chair

Sponsored by:
Membrane-Based Separations

8:00 Paper 288a: Membranes with Chemical Structure-Based Selectivity from the Assembly of Functionalizable Random Copolymer Micelles
*— **Ayse Asatekin***

8:22 Paper 288b: Fractionation of Ionic Liquid and Monomeric Sugars During Biomass Pretreatment by Nanofiltration
*— **S. Ranil Wickramasinghe**, Alexandru Avram, Xianghong Qian*

8:44 Paper 288c: Uranium-Selective Membrane Adsorbers for Use in Nuclear Forensics Applications
*— **Christine E. Duval**, Cody L. Ruff, Abenazar Darge, James C. Foster, Timothy A. DeVol, Scott M. Husson*

9:06 Paper 288d: High-Performance Separation Membranes Fabricated from Directly Synthesized MFI Nanosheets *— **Donghun Kim**, Mi Young Jeon, Prashant Kumar, Pyung-Soo Lee, Neel Rangnekar, Peng Bai, Evgenii Fetisov, Raghuram Thyagarajan, Robert F. DeJaco, Narasimharao Katabathini, Sulaiman N. Basahel, Shaeel Al-Thabaiti, K. Andre Mkhoyan, J. Ilja Siepmann, Michael Tsapatsis*

9:28 Paper 288e: Preparation and Characterization of Fluoropolymeric Microcapsules for Gas Separation Applications *— **Shayan Kaviani**, Siamak Nejati*

9:50 Paper 288f: Mixed-Matrix Membranes for Ammonium Removal from Wastewaters *— **Shu-Ting Chen**, S. Ranil Wickramasinghe, Xianghong Qian*

10:12 Paper 288g: Reliable Fabrication of Oriented Fe-MFI Membranes for Efficient Ethanol Recovery from Its Dilute Aqueous Solution
*— Xiufeng Liu, Xuguang Liu, Lin Lang, **Baoquan Zhang***, Jerry Lin*

(289) Hydrodynamics of Active Systems
Tuesday, Oct 31, 8:00 AM
Hilton, Conrad D

Ubaldo Córdova-Figueroa, Chair
Xiang Cheng, Co-Chair

Sponsored by: Fluid Mechanics

8:00 Paper 289a: Entrapment, Escape, and Diffusion of Active Particles in Complex Environments
*— **Saverio Spagnolie***

8:30 Paper 289b: Boundary Guidance in Self-Propelled Colloidal Motors
*— **Ali Mozaffari**, Joel Koplik, Charles Maldarelli*

8:45 Paper 289c: Active Nematic Liquid Crystals with Variable Activity and Elasticity *— **Rui Zhang**, Nitin Kumar, Jennifer Ross, Margaret L. Gardel, Juan de Pablo*

9:00 Paper 289d: Using a Stochastic Field Theory to Understand Active Colloidal Suspensions *— Yuzhou Qian, Peter R. Kramer, **Patrick T. Underhill***

9:15 Paper 289e: Imaging the Onset Kinetics of the Swarming Transition Using Light-Controlled Bacteria
*— **Yi Peng**, Yishu Tai, Kechun Zhang, Xiang Cheng*

9:30 Paper 289f: Surface Drag and Swarming in Motile Bacteria
*— **Pushkar Lele**, Katie Ford*

9:45 Paper 289g: Effects of Elasticity and Hydrodynamic Interactions on Swimmer Shape and Trajectories in a Coarse-Grained Model of Monotrichous Bacteria *— **Frank Nguyen**, Michael D. Graham*

10:00 Paper 289h: Microscopic Dynamics of Bacterial "Superfluids" Under Planar Oscillatory Shear
*— **Shuo Guo**, Devranjan Samanta, Yi Peng, Xinliang Xu, Xiang Cheng*

10:15 Paper 289i: Monte Carlo Simulations on the Aggregate Structures in a Suspension Composed of Magnetic Cubic Particles on a Material Surface *— **Kazuya Okada**, Akira Satoh*

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(290) IACChE's James Y. Oldshue Lecture
Tuesday, Oct 31, 8:00 AM
MCC, Ballroom B

L. Antonio Estévez, Chair

Sponsored by: Liaison Functions

8:00 Welcoming Remarks
*— **L. Antonio Estévez***

8:03 James Y. Oldshue: Life and Legacy. Lecture Series Description
*— **L. Antonio Estévez***

8:13 Speaker Introduction
*— **L. Antonio Estévez***

8:15 Paper 290a: CFD Role in Understanding Mixing Processes
*— **Jose Roberto Nunhez***

9:15 James Y. Oldshue Award Presentation

9:25 Announcements
*— **L. Antonio Estévez***

9:35 Adjourn

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(291) In-Silico Systems Biology I: Biotechnology Applications
Tuesday, Oct 31, 8:00 AM
MCC, 207A/B

Mark P. Brynildsen, Chair
Jason Shoemaker, Co-Chair
Rajib Saha, Co-Chair

Sponsored by: Bioengineering

8:00 Paper 291a: Constructing Predictive Kinetic Models of Metabolism with Transcriptional Regulation *— **Satyakam Dash**, Saratram Gopalakrishnan, Charles Foster, Costas D. Maranas*

8:18 Paper 291b: Scalable and Efficient Bayesian Metabolic Modeling with Linear-Logarithmic Kinetics
*— **Peter St. John**, Joseph Rollin, Michael F. Crowley, Yannick J. Bomble*

8:36 Paper 291c: The *E. coli* Proteome and Metallome Under Oxidative Stress
*— **Laurence Yang**, Colton J. Lloyd, Joon Ho Park, Donghyuk Kim, Sangwoo Seo, Bernhard O. Palsson*

8:54 Paper 291d: Modeling Stochasticity in the Cell Cycle
*— **Clara Hartmanshenn**, Rohit Rao, Kamau Pierre, Ioannis P. Androulakis*

9:12 Paper 291e: Application of Machine Learning and Active Learning to Enhance Chemical Yields in Microbes *— **Prashant Kumar**, Paul Adamczyk, Xiaolin Zhang, Parmeswaran Ramanathan, Jennifer Reed*

9:30 Paper 291f: In-Silico and In-Vitro Analysis of Energy Conservation and Bifurcating Enzymes in *Clostridium thermocellum* *— **Zackary Jay**, Katherine J. Chou, Kristopher A. Hunt, Maness Pin-Ching, Ross P. Carlson*

9:48 Paper 291g: Model-Guided Engineering of Microbial Biocatalysts
*— **Jennifer L. Reed***

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(292) In Honor of Bill Koros III
Tuesday, Oct 31, 8:00 AM
MCC, M100H

Ryan Lively, Chair
Mary E. Rezac, Co-Chair
John Wind, Co-Chair

Sponsored by:
Membrane-Based Separations

8:00 Paper 292a: Membranes for Separation of Complex Refinery Streams *— **Dhaval Bhandari**, Roberto Garcia, Yogesh Joshi, Marykathryn Lee, Benjamin A. McCool*

8:22 Paper 292b: Moving Towards Practical Application of Mixed-Matrix Membranes for High-Performance C_3H_6/C_3H_8 Separations *— **Jong Suk Lee***

8:44 Paper 292c: Functional Nanofiber Network Membranes for Solubility-Based Separation of Carbon Dioxide
*— **Maria R. Coleman,** Nima H. Hakim-elahi*

9:06 Paper 292d: Engineering Polymeric Hollow Fiber Contactors for Separation and Reaction Applications
*— **Ali A. Rownaghi***

9:28 Paper 292e: Real-Time Phase Imaging AFM of Palladium-Decorated Membranes for Hydrogenation
*— Matthew Young, Jared Carson, Bruce Law, Mary E. Rezac, **Peter H. Pfromm***

9:50 Paper 292f: Polycrystalline MOF Membranes on Hollow Fibers: Processing, High-Performance Separations, and Tunable Molecular Sieving *— **Sankar Nair***

10:12 Paper 292g: Advanced Functionalized Polymeric Membranes for Molecularly Selective Gas Separations *— **Shouliang Yi**, Ingo Pinnau, William J. Koros*

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(293) In Honor of Tony Cai of FRI
Tuesday, Oct 31, 8:00 AM
MCC, M100G

Daniel R. Summers, Chair
Clint P. Aichele, Co-Chair

Sponsored by:
Distillation and Absorption

8:00 Paper 293a: Bibliography of Tony Cai *— **Ken C. McCarley**, Anand N. Vennavelli, Michael R. Resetarits, Clint P. Aichele*

8:25 Paper 293b: Dr. Tony Cai's Non-Distillation Contributions to Chemical Engineering *— **Clint P. Aichele**, Michael R. Resetarits, Anand N. Vennavelli, Mason Dupre*

8:50 Paper 293c: High Energy Saving by Commercially Operated Heat-Integrated Distillation Column with New Heat Integration Arrangement
*— **Toshihiro Wakabayashi***

9:15 Paper 293d: The Relationship Between Mass Transfer Efficiency and Equilibrium in Distillation
*— **Jose Bravo***

9:40 Paper 293e: Designing Edible Oil Stripping Columns *— **Zarko Olujic**, Robin Schultz, Marlene Fuhrmeister, Helmut Jansen, Thomas Rietfort*

10:05 Paper 293f: On the Selection of Optimal Configuration for Ternary Distillation *— **Xigang Yuan**, Fang Tian, Yiqing Luo, K. T. Yu*

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(294) In Honor of Wei-Shou Hu I — 30 Years of Mammalian Cell Culture Engineering for Biologics Manufacturing (Invited Talks)
Tuesday, Oct 31, 8:00 AM
MCC, 208C/D

Weichang Zhou, Chair
James M. Piret, Co-Chair

Sponsored by:
Food, Pharmaceutical & Bioengineering Division

8:00 Introductory Remarks

8:05 Paper 294a: Professor Wei-Shou Hu: Dedicated to Service
*— **James R. Swartz***

8:25 Paper 294b: Leveraging Bioprocessing Fundamentals for the Development of Autologous Cell-Based Gene Therapies *— **Susan Abu-Absi***

8:45 Paper 294c: Opportunities and Challenges in the Commercialization of Bioproducts from Biomass and Algae
*— **George Philippidis***

9:05 Intermission

9:15 Paper 294d: Wei-Shou Hu and the Cho 'Omics Revolution
*— **Michael J. Betenbaugh***

9:35 Paper 294e: Viral Vaccines Manufacture in the Wei-Shou Hu Era
*— **John G. Aunins***

9:55 Paper 294f: An Industrial Perspective on the Impact of Cell Culture Technology Improvements on Biologics Drug Development
*— **Dana Andersen***

10:15 Comments from Wei-Shou Hu

10:25 Concluding Remarks

(295) Innovations in Production of Unconventional Reservoirs
Tuesday, Oct 31, 8:00 AM
MCC, 200B

Sandeep Verma, Chair
Sandhya Sundar Ram, Co-Chair

Sponsored by:
Upstream Engineering and Flow Assurance Forum

8:00 Paper 295a: Modeling Adsorption and Transport Processes in Kerogen — ***Gorakh Pawar***, *Hai Huang*

8:25 Paper 295b: Eagle Ford Case Study and Optimization Using Implemented Fracture Production Model — ***Xinli Jia***, *Valerij Koukhtiev, Andrey Filippov, Vitaly Khoriakov*

8:50 Paper 295c: Impact of Hydraulic Fracture Permeability on Oil Production — ***Palash Panja***, *Raul Velasco, Milind Deo*

9:15 Paper 295d: Study of Injected Water Recovery Based on New Discrete Fracture Network Approach — ***Ning Bi***, *Raul Velasco, Martin Denison, Milind Deo, John McLennan*

9:40 Paper 295e: Schlumberger's Automated Stimulation Delivery Platform — ***Rajesh Luharuka***, *Joseph P. Lima, Ann Stephen, Matthew J. Miller*

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(296) Interfacial and Nonlinear Flows: Fluid Instabilities
Tuesday, Oct 31, 8:00 AM
Hilton, Marquette I/II/III/VIII/IX

Pierre Brun, Chair
Vivek Sharma, Co-Chair

Sponsored by: Fluid Mechanics

8:00 Paper 296a: Pattern Formation from Interfacial Instabilities in Miscible Viscous Fluids — ***Irmgard Bischofberger***, *Qing Zhang*

8:30 Paper 296b: Electrokinetic Fingering: A Problem in Vector Laplacian Growth — ***Mohammad Mirzadeh***, *Martin Z. Bazant*

8:45 Paper 296c: Designing Functional Materials with Interfacial Instabilities in Thin Films — ***Pierre Brun***, *Joel Marthelot, Elizabeth Strong, Pedro Reis*

9:00 Paper 234n: Numerical Simulation on Flow Behaviour of Twin-Liquid Film over a Vertical Plate with an Open Window — ***Hanguang Xie***, *Jianguang Hu, Gance Dai*

9:15 Paper 296e: Droplet Wetting Transitions on Inclined Substrates in the Presence of External Shear and Substrate Permeability — *Leonardo Espín*, ***Satish Kumar***

9:30 Paper 296f: Measuring Contact-Line Mobility Using Drop Resonance — *Yi Xia*, ***Paul Steen***

9:45 Paper 296g: Electrostatic Suppression of the Leidenfrost State — *Arjang Shahriari*, ***Soumik Das***, *Vaibhav Bahadur, Roger T. Bonnecaze*

10:00 Paper 296h: Linear Stability of Layered Two-Phase Flow Through Soft Gel–Coated Walls — ***Dinesh N. V. S. S. R. Bhagavatula***, *S. Pushpavanam*

10:15 Paper 296i: Multiscale Analysis of a Two-Phase Flow in a Heat Exchanger Using the Wavelet Technique — *Celso Murilo dos Santos, Leonardo M. Rosa*, ***Jonathan Utzig***, *Henry F. Meier, Milton Mori*

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(297) Materials Chemistry for Biosensors
Tuesday, Oct 31, 8:00 AM
MCC, M100A

B. Reeja Jayan, Chair

Sponsored by: Sensors

8:00 Paper 297a: Point-of-Care Determining Small-Molecule Drug with Multi-Hydrogen Bonding Manipulated Single-Molecule Recognization — ***Zhe Wang***

8:20 Paper 297b: Analysis of Multiplexed Nanosensor Arrays Based on NIR Fluorescent Single-Walled Carbon Nanotubes — ***Juyao Dong***, *Michael Strano*

8:40 Paper 297c: A Biomimetic Tongue by Photoluminescent Metal–Organic Frameworks — ***Wei-Ming Chiu***, *Hung-Lin Lee, Meng-Hsun Tsai, Tu Lee*

9:00 Paper 297d: Outstanding Surface Plasmon Resonance Sensitivity and Figure of Merit Enabled by Periodic Gratings Templated from Optical Discs — ***Zhuxiao Gu***, *Peng Jiang*

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(298) Mixing in Single-Phase Systems
Tuesday, Oct 31, 8:00 AM
MCC, 102D

Clara Gomez, Chair
Richard Grenville, Co-Chair

Sponsored by:
North American Mixing Forum

8:00 Paper 298a: Investigation of Blend Time for Fully Turbulent Newtonian Fluids in Stirred Tanks — ***Aaron Strand***, *Edward Hensel*

8:19 Paper 298b: RANS-SLFM and LES-SLFM Numerical Simulations of Turbulent Non-Premixed Oxy-Fuel Jet Flames Using CO_2/O_2 Mixture — ***Adel Alghamdi***, *Rodney O. Fox, Venkat Raman, Malik Hassanaly, Yihao Tang*

8:38 Paper 298c: Effective Homogenization of Stratified Liquids Using SIDE Entry Mixing — ***Eric E. Janz***, *Kevin J. Myers*

8:57 Paper 298d: The Influence of Frame Rotation on Heat Transfer in Fully-Developed Turbulent Channel Flows — ***Charles A. Petty***, *André Bénard, Younis Najim*

9:16 Paper 298e: Counter-Rotating Vortex Shedding Generated by Acoustic Excitations in Confined Mixing Layers — *Wei Zhao*, ***Guiren Wang***

9:35 Paper 298f: Practical Large Eddy Simulation: Extension to Variable Mesh Systems — ***John A. Thomas***

9:54 Paper 298g: Species Exposure as an Approach to Quantifying Mixer Performance — ***Robert Strong***, *John A. Thomas, Markus Rumpfkeil, Eric E. Janz, Kevin Myers, Robert J. Wilkens, Minye Liu*

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(299) Model-Based Integrated Design of Pharmaceutical Drug Substance Processes I
Tuesday, Oct 31, 8:00 AM
MCC, 205A/B

Yuesheng Ye, Chair
Marimuthu Andiappan, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

8:00 Paper 299a: Intensification of a Continuous Process Guided by Mechanistic Modeling — ***Rudi Oliveira***, *Ana Cruz, Filipe Ataide, Nuno Matos*

8:25 Paper 299b: Simultaneous Estimation of Kinetic Parameters and Curve Resolution of Spectral Data: Applications and Extensions — ***Salvador García-Muñoz***, *Lorenz T. Biegler, Weifeng Chen*

8:50 Paper 299c: Modeling and Monitoring of a Continuous Silylation Reaction — ***Edward Conder***, *Carla Luciani, Jonas Y. Buser, Jeffrey Tan, Adam D. McFarland, Matthew C. Embry, Scott A. May, Mark S. Kerr, Luke Webster*

9:15 Paper 299d: Estimability Analysis for Improved Parameter Estimation in Deterministic Models: Pharmaceutical Case Studies — ***Maitraye Sen***, *Salvador García-Muñoz, Nil Tandogan, Indrakant V. Borkar, Stanley P. Kolis, Thomas M. Wilson, Jonas Y. Buser, Charles A. Alt*

9:40 Paper 299e: Solubility Data Mining and Predictive Modeling: Al+ChE — ***Jacob Albrecht***, *Jun Qiu*

10:05 Paper 299f: Toward Efficient Development and Reliable Scale-Up of Agitated Filter Drying Protocol Through DEM Modeling and Simulation — ***Kushal Sinha***, *Nandkishor Nere, John G. Gaertner, Laurie Mlinar, Raimundo Ho, Alessandra Mattei, Haojuan Wei, Samrat Mukherjee, Ahmad Sheikh, Shailendra Bordawekar*

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(300) Multiscale Systems Engineering I — In Honor of Professor Christodoulos A. Floudas (Invited Talks)
Tuesday, Oct 31, 8:00 AM
MCC, 103C

Efstratios N. Pistikopoulos, Chair
Marianthi Ierapetritou, Co-Chair
Costas D. Maranas, Co-Chair

Sponsored by:
Computing Systems and Technology Division

8:00 Opening Remarks — ***Costas D. Maranas***

8:05 Paper 300a: BASBL: Branch-and-Sandwich Bilevel Solver — Implementation and Computational Study Using BASBLib Test Set — *Remigijus Paulavicius*, ***Claire S. Adjiman***

8:22 Paper 300b: Highly Efficient Consolidated Bioprocessing of Lignocellulose into Biofuels and Bioproducts: Integrating Cellular and Process Systems Engineering — ***Xiaoxia (Nina) Lin***

8:39 Paper 300c: Robust Optimization for Problems with Endogenous Uncertainty — *Nikolaos Lappas*, ***Chrysanthos E. Gounaris***

8:56 Paper 300d: Heuristics with Performance Guarantees for the Minimum Number of Matches in Heat Recovery Networks — *Georgia Kouyialis, Dimitrios Letsios*, ***Ruth Misener***

9:13 Paper 300e: Recent Contributions by Floudas Lab at the Interface of Chemical Engineering and Computational Biology — ***George A. Khoury***

9:30 Paper 300f: Advances in Modeling, Synthesis, and Global Optimization of Hybrid Energy Systems — ***Onur Onel***, *Alexander M. Niziolek, Christodoulos A. Floudas*

9:47 Paper 300g: Circadian Entrainment and Synchronization in Health and Disease: A Tail of Many Rhythms — ***Ioannis P. Androulakis***

10:04 Paper 300h: On a Mathematical Modelling and Optimization Approach for the Systematic Synthesis and Development of Integrated Value Chains for Biorefineries — ***Antonis C. Kokossis***

10:21 Concluding Remarks

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(301) Nanomaterials for Energy Storage
Tuesday, Oct 31, 8:00 AM
MCC, 200G

Yong L. Joo, Chair
Yu-Sheng Su, Co-Chair

Sponsored by:
Nanomaterials for Applications in Energy and Biology

8:00 Paper 301a: Controllable Hydrothermal Conversion from Ni-Co-Mn Carbonate Nanoparticles to Spheres — ***Yanqing Tang***, *Lu Yangcheng, Luo Guangsheng*

8:20 Paper 301b: Oxidative Chemical Vapor Deposition of Polyaniline: Influence of Process Conditions on Film Chemistry and Electrochemical Performance — *Yuriy Y. Smolin*, ***Xiaobo Li***, *Kenneth K. S. Lau*

8:40 Paper 301c: High-Performance Pillared V_2O_5 and MnO_2 Cathodes for Lithium-Ion Batteries — ***Yixuan Chen***, *Siu on Tung, Krista L. Hawthorne, Woo-ram J. Lee, Levi T. Thompson*

9:00 Paper 301d: 2D Transition Metal Carbides (MXenes): Synthesis and Applications in Electrochemical Energy Storage — ***Mengqiang Zhao***, *Chang E. Ren, Babak Anasori, Yury Gogotsi*

9:20 Paper 301e: Design, Synthesis, and Characterization of Mixed Ionic/Electronic Conducting Surface Layers Adsorbed on Metal Oxide Particles — ***Jeffrey J. Richards***, *Norman Wagner, Paul Butler*

9:40 Break

10:00 Paper 301g: Conductive Membrane Coatings for Improving Current Density in Redox Flow Batteries — ***Andrew Shah***, *Yong Lak Joo*

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(302) Nanoparticles and Health
Tuesday, Oct 31, 8:00 AM
MCC, 210A/B

Kerry Kelly, Chair
Nga Lee Ng, Co-Chair

Sponsored by:
Environmental Aspects, Applications, and Implications of Nanomaterials and Nanotechnology

8:00 Paper 302b: Soot Source Identification by Laser Derivatization — ***Madhu Sing***, *Randy Vander Wal*

8:20 Paper 302c: Evaluation of Biological Effects Using a Nano-Ceria-Based Diesel Fuel Additive with In-Vitro Air-Liquid Interface Cell Exposure Systems of Different Flow Patterns — ***Lynn E. Secondo***, *Penelope K. Baltzopoulou, Akrivi Asimakopoulou, Daniel Deloglou, Christos Softas, Spyros Petrakis, Leonidas Chasapidis, Eleni Papaioannou, Athanasios G. Konstandopoulos, Nastassja Lewinski*

8:40 Paper 302f: Oxidative Stress Induced by Ambient Air PM_x: Which Are the Main Sources? — *Marianthi Kermenidou*, ***Spyros Karakitsios***, *Dimosthenis Sarigiannis*

9:00 Paper 302d: Development of Predictive Tools for Aviation Non-Volatile Particulate Emissions — ***Joseph Abrahamson***, *Vander Wal Randy*

9:20 Paper 302e: Molecular Initiating Events Linked to Carbon Nanotube Functionalization for Medical Applications — ***Dimosthenis Sarigiannis***

9:40 Paper 302g: Effect of Combustion Particle Size on Pathologically Important Responses in Lung Cells — *Kamaljeet Kaur, Raziye Mohammadpour, Isabel Jaramillo, Robert Paine, Christopher Reilly, Hamid Ghandehari*, ***Kerry Kelly***

10:00 Paper 302a: Oxidative Stress Induced by Secondary Organic Aerosols (SOA) Generated from Biogenic and Anthropogenic Precursors — *Wing-Yin Tuet, Yunle Chen, Shierly Fok, Julie A. Champion*, ***Nga Lee Ng***

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(303) Nanoscale Structure in Polymers
Tuesday, Oct 31, 8:00 AM
MCC, 211C

Shudipto Konika Dishari, Chair
Jian Qin, Co-Chair

Sponsored by: Polymers

8:00 Paper 303a: Tapered Block Copolymers: Tuning Self-Assembly and Properties by Manipulating Monomer Segment Distributions — ***Thomas H. Epps, III***

8:30 Paper 303b Photoplasiticity in Crosslinked Liquid Crystalline Networks: A Route to Reconfigurable Shape-Changing Materials — ***Matthew K. McBride***, *Matthew Hendrikx, Danqing Liu, Brady Worrell, Dick J. Broer, Christopher Bowman*

8:45 Paper 303c: Synthesis of Novel Nanostructured Copolymers with Alternating Linear Polymer and Dendrimer Blocks — ***Haotian Sun***, *Alex Commisso, Chong Cheng*

9:00 Paper 303d: Hierarchical Structures of PDMS-PU Copolymer and Particles for Hydrophobic Coatings — ***Marius Rutkevicius***, *Mackenzie Geiger, Tahira Pirzada, Saad A. Khan*

9:15 Paper 303e: Charged Polymer Conformations in Polyelectrolyte Complexes — ***Amanda B. Marciel***, *Samanvaya Srivastava, Matthew V. Tirrell*

9:30 Paper 303f: Solubility Parameters, Water Activity Coefficients and Proton Mobility of Sulfonated Poly(styrene-isobutylene-styrene), Sulfonated Poly(ether ether ketone), and Sulfonated Poly(2-ethoxyethyl methacrylate) Membranes — ***Maritza Perez Perez***, *David Suleiman*

9:45 Paper 303g: Single-Molecule Super-Resolution Microscopy in Nanostructured Polymer Thin Films — ***Muzhou Wang***, *James M. Marr, Jeffrey W. Gilman, J. Alexander Liddle*

10:00 Paper 303h: A Non-Equilibrium Molecular Dynamics (NEMD) Simulation of the Crosslinked Polyamide Membrane in Water Desalination — ***Md. Symon Jahan Sajib***, *Tao Wei*

10:15 Paper 303i: Continuous Synthesis Process of Polyimide Sponge and Its Pore Size Control — ***Gunhwi Kim***, *Jinyoung Kim, Daero Lee, Haksoo Han*

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(304) New Developments in Computational Catalysis I
Tuesday, Oct 31, 8:00 AM
MCC, L100E

Heather J. Kulik, Chair
Shaama Mallikarjun Sharada, Co-Chair
Bin Liu, Co-Chair
Eric Walker, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

8:00 Paper 304a: Multiconfiguration Pair-Density Functional Theory for Computational Catalysis — ***Laura Gagliardi***, *Donald G. Truhlar*

8:31 Paper 304b: Quantum-Mechanical Description of Excited-State Heterogeneous Catalysis via Embedded Correlated Wavefunction Methods — ***John Mark P. Martirez***, *Emily A. Carter*

8:48 Paper 304c: Incorporation of Linear Scaling Relations into Automatic Mechanism Generation for Heterogeneous Catalysis — ***Richard H. West***, *C. Franklin Goldsmith*

9:05 Paper 304d: DFT+U-Inspired Functional for Improved Modeling of Molecules and Solids — ***Alexander V. Mironenko***, *Dionisios G. Vlachos*

9:22 Paper 304e: Development of "Surrogate" Hybrid Functionals Based on Electron Density Convolutions — ***Andrew Medford***, *Ray Lei*

9:39 Paper 304f: Accurate Correction of DFT Delocalization Error in Transition Metal Catalysis — ***Qing Zhao***, *Terry Z. H. Gani, Akash Bajaj, Heather J. Kulik*

9:56 Paper 304g: The Effects of Oxidation and Transition Metal Doping on the Structure and Properties of Pt-Ni Nanoparticles — ***Liang Cao***, *Tim Mueller*

10:13 Paper 304h: The Influence of Hubbard U Parameter in Simulating Adsorption and Reactivity on CuO Surface(s): A Combined Theoretical and Experimental Study — ***Kartavya Bhola***, *Jithin John Varghese, Liu Dapeng, Yan Liu, Samir H. Mushrif*

TECHNICAL SESSIONS 2017

(305) New Frontiers of Molecular Thermodynamics (Invited Talks)
Tuesday, Oct 31, 8:00 AM
MCC, L100J

Rajesh Khare, Chair
Shekhar Garde, Co-Chair

Sponsored by:
Thermodynamics and Transport Properties

8:00 Paper 305a: Inverse Design of Interactions for Assembly
— ***Thomas M. Truskett***

8:30 Paper 305b: High-Throughput Computational Screening as a Tool for Understanding the Molecular Thermodynamics of Adsorption
— ***Randall Q. Snurr***

9:00 Paper 305c: Awe-Somes: All Water Emulsion Bodies
— ***Kathleen J. Stebe***, *Sarah Hann, Daeyeon Lee*

9:30 Paper 305d: Succession of Alkane Conformational Motifs Bound Within Hydrophobic Nano-Capsule Assemblies — ***Hank Ashbaugh***

10:00 Paper 305e: Thermodynamics and Transport Properties of Fluids with Intermediate Range Order with Application to Protein Solutions and Biopharmaceuticals — *P. Douglas Godfrin, Yun Liu, Nestor Valadez, Ramon Castaneda-Priego, Jonas Riest, Gerhard Naegele,* ***Norman Wagner***

(306) Polymer Processing and Rheology
Tuesday, Oct 31, 8:00 AM
MCC, 211D

Amy M. Peterson, Chair
Vivek Sharma, Co-Chair
Rohan Hule, Co-Chair

Sponsored by: Polymers

8:00 Paper 306a: Linear and Nonlinear Rheology Predictions of Entangled Polymers in Complex Flows from First Principles — ***Jay D. Schieber***

8:30 Paper 306b: Melt Behavior-Chain Architecture-Polymer Composition Correlations in High-Density Polyethylene — ***Rohan Hule***, *Derek W. Thurman, Antonios Doufas*

8:45 Paper 306c: Shear-Induced Conformational Changes of Flexible and Semi-Rigid Engineering Thermoplastics and Their Influence on Crystallization
— ***Behzad Nazari***, *Jiho Seo, Ralph H. Colby, Alicyn M. Rhoades, Richard P. Schaake*

9:00 Paper 306d: Island-in-the-Sea Meltblown Nanofiber Nonwovens with Diverse Surface Properties for Filtration Applications — ***Iman Soltani***, *Satish Kumar, Frank S. Bates, Christopher W. Macosko*

9:15 Paper 306e: Enthalpic and Entropic Competitions in Solvent-Free Polymer-Grafted Nanoparticles
— ***Snehashis Choudhury***, *Lynden A. Archer*

9:30 Paper 306f: Designing Material Dynamics in Polyelectrolyte Complexes — ***RZdeg Ebn***, *Brian Momani, Matthew Labbe, H. Henning Winter, Sarah L. Perry*

9:45 Paper 306g: Extensional Relaxation Times of Dilute and Semi-Dilute Polymer Solutions
— *Jelena Dinic, Leidy N. Jimenez, Madeleine Biagioli,* ***Vivek Sharma***

10:00 Paper 306h: Nonequilibrium Molecular Dynamics Simulations of Entangled Polymer Solutions Undergoing Planar Elongational Flows — ***Mohammad Hadi Nafar Sefiddashti***, *Brian J. Edwards, Bamin Khomami*

10:15 Paper 306i: Ultra-High-Performance Polymers Meet Ionic Liquids — ***Jason E. Bara***, *Kathryn O'Harra, Grayson P. Dennis, Marlow M. Durbin, Max Mittenthal, Enrique M. Jackson*

(307) Process Intensification and Integration of Water and Energy Usage
Tuesday, Oct 31, 8:00 AM
MCC, 101D

Tracy J. Benson, Chair
Peyman Fasahati, Co-Chair

Sponsored by:
Sustainable Biorefineries

8:00 Paper 307a: IGCC Process Intensification with the Reforming Technologies for Enhanced Power Generation with CCS Technology — ***Usama Ahmed***, *Younggeun Lee, Seolin Shin, Umer Zahid, Chonghun Han*

8:22 Paper 307b: Vegetable Oil Process Intensification with Sterically Hindered Alcohols to Biofuels and Biochemicals — ***Daria C. Boffito***, *Federico Galli, Kieran Horry, Gregory Patience*

8:44 Paper 307c: Targeting Maximum Energy and Water Efficiencies for the Sustainable Total Textile Waste Refinery
— ***Athanassios Nikolakopoulos***, *Foteini Barla, Antonis C. Kokossis*

9:06 Paper 307d: Advances in Process Intensification: Using Reactive Distillation for the Conversion of Crude Glycerol — ***Obakore Agbroko***, *Tracy J. Benson*

9:28 Break

9:50 Paper 307f: Process Design and Techno-Economic Assessment of a Seaweed-Based Biorefinery: Integration of Thermochemical and Biochemical Conversion Processes
— ***Boris Brigljevic***, *J. Jay Liu*

10:12 Paper 307g: Process Intensification and Modularization for Sustainability — ***Dion G. Vlachos***

(308) Reaction Chemistry and Engineering I
Tuesday, Oct 31, 8:00 AM
MCC, L100B

Klavs F. Jensen, Chair
Saif A. Khan, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

8:00 Paper 308a: Application of Structured Porous Reactors for Heat-Sensitive Liquid-Liquid Reactions
— *Aditi Potdar, Leen C. J. Thomassen,* ***Simon Kuhn***

8:22 Paper 308b: Heterogeneous Interfaces Confined in Microreactors and Characterized by *In-Situ* Spectroscopic Techniques
— *Bruno Pinho, Karishma Minsariya, Weiqi Chen,* ***Ryan L. Hartman***

8:44 Paper 308c: Reaction Mechanism and Microkinetics of the Cobalt-Catalyzed Fischer–Tropsch Synthesis
— ***G. T. Kasun Kalhara Gunasooriya***, *Mark Saeys*

9:06 Paper 308d: Interplay of Reaction and Transport Within Biomass Particle During Fast Pyrolysis: Development of Reaction and Transport Models and Their Non-Dimensionalization
— ***Khursheed B. Ansari***, *Samir H. Mushrif, Daniel V. Viju, Nasser M. Abukhdeir, Saurabh Maduskar, Paul J. Dauenhauer*

9:28 Paper 308e: Kinetics of Glycerol Conversion to Hydrocarbon Fuels over Pd/H-ZSM-5 Catalysts — ***Yang Xiao***, *Arvind Varma*

9:50 Paper 308f: Reaction of C2H4 Under Lower-Temperature Fischer-Tropsch Conditions on a TiO2-Supported Cobalt Catalyst with Co-Feeding of H2 and Syngas
— ***Xiaojun Lu***, *Diane Hildebrandt, Xinying Liu, Yusheng Zhang*

10:12 Paper 308g: High-Throughput Study of Catalysis on Pd-Based Alloys
— ***Irem Sen***, *Xiaoxiao Yu, Petro Kondratyuk, Andrew J. Gellman*

(309) Scholarship of Teaching and Learning, and Assessment
Tuesday, Oct 31, 8:00 AM
MCC, 205C

Laura Ford, Co-Chair
Kevin Hadley, Co-Chair

Sponsored by:
Undergraduate Education

8:00 Introductory Remarks

8:01 Paper 309a: What Is the Scholarship of Teaching and Learning?
— ***Laura Ford***

8:11 Paper 309b: Design Challenge Parleys as a Conduit for Growing Student Expert Thinking in the Classroom — ***Jamie Gomez***, *Vanessa Svihla, Abhaya K. Datye, Victor Law, Sophia Bowers*

8:31 Paper 309c: Course Design vs. Student Experience: To What Extent Do We Agree on What Happens in Class?
— ***Margot Vigeant***, *Michael Prince, Erin Jablonski, Katharyn Nottis, Amy Golightly*

8:51 Paper 309d: A Longitudinal Study Regarding the Impact of a Teamwork Skill-Building Activity — ***Kevin Hadley***, *Ken Reid*

9:11 Paper 309e: Identifying Factors That Aid Students in Developing "Engineering Intuition"
— ***Elif E. Miskioglu***, *Kaela Martin*

9:31 Assessment

9:32 Paper 309f: Using Survey Data to Assess Chemical Engineering Student Acumen — ***Matthew Armstrong***, *Geoffrey Bull, Andrew Biaglow*

9:52 Paper 309g: Using E-Portfolios to Assess ABET Outcomes and Student Learning — ***Tracy Carter***, *Ronald J. Willey*

10:12 Panel Discussion

(310) Solid Form Selection: Cocrystals, Salts, Solvates, Polymorphs, and Beyond
Tuesday, Oct 31, 8:00 AM
MCC, M100J

Fang Wang, Chair
Meenesh R. Singh, Co-Chair

Sponsored by:
Crystallization and Evaporation

8:00 Introductory Remarks

8:05 Paper 310a: A Novel Microfluidic Platform for Screening of Pharmaceutical Polymorphs Under Hydrodynamically Controlled Crystallization Conditions
— ***Paria Coliaie***, *Meenesh Singh*

8:25 Paper 310b: Polymorphism in Drug Compounds by Controlling Fluid Dynamics During Crystallization
— ***Stephanie Guthrie***, *Gaurav Giri*

8:45 Paper 310c: Crystal Form Conversion of Cyantraniliprole by Extruding Powder
— ***Daniel A. Green***, *Matthew R. Oberholzer, Marios Avgousti, William Wilkins, Victoria Lai*

9:05 Paper 310d: Continuous Cocrystallization of Benzoic Acid and Isonicotinamide by Mixing-Induced Supersaturation: Exploring Opportunities Between Reactive and Antisolvent Crystallization Concepts
— ***Vaclav Svoboda***, *Pól MacFhionnghaile, John McGinty, Lauren E. Connor, Iain D. H. Oswald, Jan Sefcik*

9:25 Paper 310e: A Multiscale Computational Method for Prediction of Polymorphs — ***Anish V. Dighe***, *Meenesh R. Singh*

9:45 Paper 310f: Polymorph Selection by Continuous Precipitation
— ***Thomas Farmer***, *Sina Schiebel, Bradley F. Chmelka, Michael F. Doherty*

10:05 Paper 310g: Mechanism of Selective Co-Crystallization of Cresol Isomers with Urea — ***Na Wang***, *Hongxun Hao, Qiuxiang Yin, Baohong Hou, Meijing Zhang*

10:25 Concluding Remarks

(311) Solids Handling and Processing II
Tuesday, Oct 31, 8:00 AM
MCC, 200J

Gary Liu, Chair
Csaba Sinka, Co-Chair

Sponsored by:
Solids Flow, Handling and Processing

8:00 Paper 311a: Prediction of Bulk Solid Properties of Formulations
— ***Madhusudhan Kodam***, *Karl Jacob, Jaime Curtis-Fisk, Karen Balwinski, Andrew Horton, Michael Zink*

8:18 Paper 311b: Extension of a Mechanistic Model for Drying of Single Pharmaceutical Granules to Semi-Continuous Fluid Bed Drying
— ***Michael Ghijs***, *Séverine T. F. C. Mortier, Philippe Cappuyns, Krist V. Gernaey, Thomas De Beer, Ingmar Nopens*

8:37 Paper 311c: Impregnation of Metal Solutions in Catalytic Porous Particles and Axial Dispersion Studies in Rotating Drum Using Experiments and DEM Simulations
— *Yangyang Shen, William G. Borghard,* ***M. Silvina Tomassone***

8:56 Paper 311d: Performance Evaluation of Vacuum and Positive-Pressure System for Dilute-Phase Pneumatic Conveying of Barium Sulfate
— ***Amit K. Gautam***, *Jason Brantley, Johnselvakumar Lawrence*

9:15 Paper 311e: Impact of Microwave and Other Drying Techniques on the Dissolution Bioavailability of Naproxen Sodium Drug — ***Maha AL-ALI***, *Selvakannan Periasamy, Rajarathinam Parthasarathy*

9:34 Paper 311f: Swirl Number Analysis for Performance Data Prediction of Uniflow Cyclones
— ***Martin Pillei***, *Tobias Kofler, Michael Kraxner*

9:53 Paper 311g: Saponin Removal from Bitter Quinoa Ecotypes in Spouted Beds (SB) — ***Carlos Ramiro Escalera***, *Carmen Carla Quiroga Ledezma, Luis Arteaga Weill*

10:12 Paper 311h: Influence of the Viscosity on the Velocity Propagation in Axial Direction in a Rietema Hydrocyclone — ***Thomas Senfter***, *Martin Pillei, Manuel Berger, Anke Bockreis, Wolfgang Rauch, Michael Kraxner*

(312) Steal This Activity/ Demonstration/Assignment
Tuesday, Oct 31, 8:00 AM
MCC, 205D

Daniel D. Burkey, Co-Chair
Matthew Cooper, Co-Chair
Shannon Ciston, Co-Chair

Sponsored by: Undergraduate Education

8:00 Paper 312a: A 'Cards Against Humanity'-Style Card Game for Increasing Engineering Students' Awareness of Ethical Issues in the Profession — ***Daniel D. Burkey***, *Michael Young, Landon Bassett*

8:20 Paper 312b: Incorporating Diversity and Bias Awareness in a Technical and Professional Communication Course
— ***Elif E. Miskioglu***

8:40 Paper 312c: Providing Access to Clean Water: Activities for Freshman Engineering Courses and Outreach
— ***Virginia Davis***, *Joni Lakin, Edward W. Davis*

9:00 Paper 312d: Supplement Homework with Problems from a Freely Available Repository — ***John Wagner***, *Allen Hersel, Amanda P. Malefyt*

9:20 Paper 312e: Liquid-Liquid Extraction: Last but Not Least
— ***Timothy Threatt***, *Jacob H. Arredondo, Jonathan H. Worstell*

9:40 Paper 312f: Portable Wet Process Control Laboratory for Every Student's Desk and Home — ***Spyros Svoronos***

10:00 Paper 312g: Vertically Integrated IoT, Off-Grid Control Sensors, Advancing with Arduino, Android App Shells, Programming, Rapid Big Data: The Kitchen Sink — ***Cory Jensen***

(313) Sustainable Fuel from Renewable Resources
Tuesday, Oct 31, 8:00 AM
MCC, 102E

Jeffrey Seay, Chair

Sponsored by: Sustainability

8:00 Paper 313a: Low-Temperature Catalytic Gasification of Particulate Waste Materials — ***Uchechukwu Obiako***, *Eric M. Lange, Samuel Sanya, Jorge E. Gatica*

8:20 Paper 313b: Experimental Analysis of Catalytic Gasification of Waste Polymers — ***Samuel Sanya***, *Uchechukwu Obiako*

8:40 Paper 313c: Intensification of Enzymatic Hydrolysis of Cellulose to Glucose by High-Frequency Ultrasound: Optimization of Process Parameters and Effects on Enzyme Stability
— ***Yusuf G. (Debo) Adewuyi***

9:00 Paper 313d: Catalytic Gasification: A Sustainable Waste Management Alternative
— *Eric M. Lange,* ***Uchechukwu Obiako***, *Samuel Sanya, Stephen A. Reeves, Aliandra D. Barbutti, Jorge E. Gatica*

9:20 Paper 313e: Energy Performance of an Integrated Biomass Gasification and SOFC Combined-Cycle Power Plants with CO2 Capture
— ***Po-Chih Kuo***, *Wei Wu*

9:40 Paper 313f: Pyrolysis of Food Waste: Thermal Deconstruction Rates in a Regular Calcination Oven vs. an Induction Heating Reactor
— *Cosmin Marculescu, Raluca-Nicoleta Tirtea, Aurelia-Iustina Stanciulescu,* ***Dorin Boldor***

(314) Sustainable Management of Post-Consumption/Use Biomaterials
Tuesday, Oct 31, 8:00 AM
MCC, 101C

Jason Trembly, Chair
Gerardo J. Ruiz-Mercado, Co-Chair

Sponsored by: General

8:00 Paper 314a: Hydrothermal Carbonization of Wastes for Simultaneous Nutrient Recovery and Energy Capture — ***Charles Coronella***, *Saeed Vahed Qaramaleki, Sage R. Hiibel, Silvia Román, Nicholas Silva*

8:25 Paper 314b: Using Fly Ash as pH Adjustment for Efficient Phosphorus Immobilization and Reutilization from Swine Manure in Hydrothermal Treatment — ***Jason Trembly***, *Wen Fan*

8:50 Paper 314c: Recovery of High-Value Chemicals from Organic Waste: Economic Potential and Logistical Issues — ***Yicheng Hu***, *Daniel Noguera, Victor M. Zavala*

9:15 Paper 314d: Optimization of Biorefinery Production Chains and Decision-Making Through Sustainability Evaluation: A Biojet Fuel Case Study
— ***Ana I. Torres***, *Eduardo Vyhmeister, Gerardo J. Ruiz-Mercado, John A. Posada*

9:40 Paper 314e: Eco-LCA Methodology for Sustainability Assessment of Bio-WWTS Focused on Energy Recovery
— ***Alexander Meneses-Jácome***, *Ángela Adriana Ruiz-Colorado*

10:05 Paper 314f: Sustainability Assessment Water Resources Use Mining in Colombia, by the Emergy Analysis — ***Natalia Andrea Cano***, *Hector Ivan Velásquez, Oswaldo Bustamente*

(315) Symposium on Solar Power and Chemical Systems in Honor of Prof. Edward A. Fletcher I
Tuesday, Oct 31, 8:00 AM
MCC, 201A/B

Wojciech Lipinski, Chair
Nick AuYeung, Co-Chair
Alexandre Yokochi, Co-Chair

Sponsored by:
Symposium on Solar Power and Chemical Systems in Honor of Prof. Edward A. Fletcher

8:00 Paper 315a: Keynote — Jet Fuel from H_2O, CO_2, and Solar Energy
— ***Aldo Steinfeld***

8:30 Paper 315b: The Role of Charge-Compensating Dopants in Decreasing the O-Vacancy Formation Energy in Ceria — ***Christopher L. Muhich***, *Marie Hoes, Aldo Steinfeld*

8:50 Paper 315c: Redox-Active $Y_{0.5}Ba_{0.5}Co_{03-\delta}$ as Thermochemical Oxygen Pump for O_2-Inert Gas Separations — ***Ronald Michalsky***, *Miriam Ezbiri, Aldo Steinfeld*

9:10 Paper 315d: Reduction Kinetics of Hercynite ($FeAl_2O_4$) and Hydrogen Production for Solar Thermochemical Water Splitting
— ***Ibraheam Al-Shankiti***, *Hicham Idriss, Alan W. Weimer*

9:30 Paper 315e: Near-Isothermal On-Sun Demonstration to Split Water — ***Amanda Hoskins***, *Samantha L. Millican, Caitlin Czernik, Mark Wallace, Ibraheam Al-Shankiti, Judy Netter, Charles B. Musgrave, Alan W. Weimer*

9:50 Paper 315f: Solar Thermochemical Fuel Production in a Microreactor — ***Fuqiong Lei***, *Yige Wang, Thana Sornchamni, Nuchanart Siri-Nguan, Goran Jovanovic, Liney Arnadottir, Alexandre Yokochi, Unalome Wetwatana-Hartley, Nick AuYeung*

10:10 Paper 315g: Reactor Design and Evaluation for the Solar Photo-Thermochemical Processing of Carbon Dioxide and Methane — ***Saroj Bhatta***, *Juan P. Trelles*

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(316) Synthetic Biology Applications I: Human Health and Disease
Tuesday, Oct 31, 8:00 AM
MCC, 208A

Ian Wheeldon, Chair
Keith E. J. Tyo, Co-Chair

Sponsored by: Bioengineering

8:00 Paper 316a: Metabolic Engineering and Synthetic Biology with Human Milk Oligosaccharides — ***Fatima Enam***, *Yanfen Bai, Thomas J. Mansell*

8:18 Paper 316b: Engineered Probiotics for the Treatment of Multidrug-Resistant *E. coli* — ***Brittany Forkus***, *James Johnson, Yiannis Kaznessis*

8:36 Paper 316c: Synthetic RNA-Inhibitor Antibiotics in Non-Traditional Antibiotic Pathways to Treat Multi-Drug-Resistant Bacteria — ***Colleen Courtney***, ***Anushree Chatterjee***

8:54 Paper 316d: Optogenetic Regulation of Insulin Secretion in Pancreatic Beta-Cells — *Fan Zhang,* ***Emmanuel S. Tzanakakis***

9:12 Paper 316e: An Oncogene Activity-Dependent "Suicide Gene" Vector System for Selective Targeting of Cancer Cells — ***Evan K. Day***, *Ashley E. Pandolf, Matthew J. Lazzara*

9:30 Paper 316f: Genetically Encoded, Synthetic Glycopolymers for Tunable Control of Plasma Membrane Shapes and Organelle Biogenesis — ***Carolyn Shurer***, *Marshall Colville, Joe C-H. Kuo, LaDeidra Roberts, Hao Pan, Jay Gandhi, Matthew Paszek*

9:48 Paper 316g: Enabling Design-Driven Medicine with Synthetic Biology: Engineering Programmable Cell-Based Therapies — ***Joshua N. Leonard***

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(317) The Energy-Water Nexus
Tuesday, Oct 31, 8:00 AM
MCC, 102A

Urmila M. Diwekar, Chair
Shweta Singh, Co-Chair

Sponsored by: Sustainable Energy

8:00 Paper 317a: Thermodynamic Analysis of an Ion-Exchange-Based Waste Water Treatment for Phosphorus Recovery — ***Gargeya Vunnava***, *Shweta Singh*

8:20 Paper 317b: Shale Gas Wastewater Management Using Membrane Distillation: An Optimization-Based Approach — ***Sakineh Tavakkoli***, *Omkar Lokare, Radisav D. Vidic, Vikas Khanna*

8:40 Paper 317c: Systematic Analysis and Optimization of Water-Energy Nexus — ***Spyridon D. Tsolas***, *M. Nazmul Karim, M. M. Faruque Hasan*

9:00 Paper 317d: Biologically Active Filters: A Sustainable Treatment Process for Emerging Contaminants — ***Lisa Axe***, *Shuangyi Zhang, Stephen Gitungo, Robert Raczko, Sophie Courtois, John Dyksen*

9:20 Paper 317e: Optimal Design of Macroscopic Water-Energy Networks Under Uncertainty — ***Rajib Mukherjee***, *Nasreen A. Elsayed, Ramon Gonzalez-Bravo, Jose Maria Ponce-Ortega, Patrick Linke, Mahmoud M. El-Halwagi*

9:40 Paper 317f: Water Expulsion from Carbon Rods at High Humidity — ***Satish K. Nune***, *David J. Heldebrant, David Lao, Matthew Olszta, Yongsoon Shin, Xiao-Ying Yu, Juan Yao*

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(318) Topical Plenary: Award Speaker Session for Green Process Engineering (Invited Talks)
Tuesday, Oct 31, 8:00 AM
MCC, 103A

Yizu Zhu, Chair
Jian Liu, Co-Chair
Wei Liu, Co-Chair

Sponsored by: Innovations of Green Process Engineering for Sustainable Energy and Environment

8:00 Paper 318a: Advanced Membranes for PM2.5 Filtering, Ethanol Dehydration, and Air Dehumidification — ***Wei Liu***

8:25 Paper 318b: Large-Scale Removal of Atmospheric CO_2 Through Biomass Chemical-Looping Combustion — ***Kevin Whitty***

8:50 Paper 318c: Greener Processing for the Conversion of Waste Plastics into Energy-Storing Carbons — ***Vilas G. Pol***

9:15 Paper 318d: Green Process Engineering: Fundamental Researches and Applications of Ionic Liquids — ***Suojiang Zhang***

9:40 Paper 318e: Unlocking Biomass Energy: Process Development and Scale-Up of Biomass Conversion to Advanced Fuels and Chemicals — ***Ning Sun***

10:05 Paper 318f: Completing the New Biofuel and Bio-Derived Chemicals and Materials Research Challenge — ***Arthur J. Ragauskas***

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(319) Topical Plenary: Chemical Engineers in Medicine II (Invited Talks)
Tuesday, Oct 31, 8:00 AM
MCC, 202A/B

Swomitra Mohanty, Chair
Leonard F. Pease III, Co-Chair

Sponsored by: Chemical Engineers in Medicine

8:00 Paper 319a: Producing Protein Therapeutics Without Cells — ***Bradley C. Bundy***

8:40 Paper 319b: In-Situ Thermal Eradication of Biofilms — ***Eric Nuxoll***

9:20 Paper 319c: Single-Use Sensor Array for Monitoring Key Growth Medium Analytes During mAbs Biomanufacturing — ***Jules Magda***

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(320) Tutorial Session on Electrochemical Methods, Systems and Applications (Invited Talks)
Tuesday, Oct 31, 8:00 AM
MCC, M100C

Fikile Brushett, Chair
Daniel V. Esposito, Co-Chair
Thomas F. Fuller, Co-Chair
John Harb, Co-Chair

Sponsored by: Electrochemical Fundamentals

8:00 Paper 320d: 20 Years of Corrosion Sensing and Microvisualization of Corrosion Processes — ***William H. Smyrl***

8:35 Paper 320a: The Need for Engineering Methods for Electrochemical Systems — ***Richard Alkire***

9:10 Break

9:20 Paper 320b: Characterizing Metal-Air Batteries Using Electrochemical Impedance Spectroscopy and Mass Spectrometry — ***Bryan D. McCloskey***

9:55 Paper 320c: Platinum-Free Fuel Cells for Affordable Zero-Emission Cars — ***Yushan Yan***

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(321) Using the Brains of Others to Innovate Faster
Tuesday, Oct 31, 8:00 AM
MCC, L100G

Jack Hipple, Chair

Sponsored by: Professional Development

8:00 Paper 321a: Using a Structured Approach to Efficiently Use the Brains of Others to Make Problem Solving More Productive — ***Jack Hipple***

10:05 Paper 321b: AIChE Engage: Your Next Stop for Brainstorming in the Process of Problem Solving or Innovating — ***Tianxing Cai***

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(322) Value-Added Chemicals from Natural Gas
Tuesday, Oct 31, 8:00 AM
MCC, 200C

Dushyant Shekhawat, Chair
Götz Veser, Co-Chair
John Hu, Co-Chair

Sponsored by: Advances in Fossil Energy R&D

8:00 Paper 322a: Catalyst Development for Natural Gas Monetization — ***Jonas Baltrusaitis***, *Israel E. Wachs, Zili Wu, Minghui Zhu, Michael Ford, William Taifan, Lohit Sharma*

8:19 Paper 322b: Mechanistic Insight for Oxidative Coupling of Methane on Mg6MnO8-Based Redox Catalysts in a Chemical-Looping System — ***Deven Baser***, *Zhuo Cheng, Sourabh Nadgouda, Lang Qin, Liang-Shih Fan*

8:38 Paper 322c: Gold-Palladium Particle Size Effect on Methane Oxidation Activity — ***Christopher Williams***, *James H. Carter, Nicholas F. Dummer, Robert Armstrong, Sara Yacob, David Willock, Randall J. Meyer, Stuart H. Taylor, Graham J. Hutchings*

8:57 Paper 322d: Printable Bioreactors for Bioconversion of Methane to Value-Added Chemicals — ***Jennifer M. Knipe***, *Sarah E. Baker*

9:16 Paper 322e: Influence of Platinum on the Activity of Ga/HZSM-5 Catalyst in Ethane Dehydroaromatization Reaction — ***Anupam Samanta***, *Xinwei Bai, Brandon Robinson, Dushyant Shekhawat, John Hu*

9:35 Paper 322f: Dehydroaromatization of Methane to Benzene, Toluene and Naphthalene in a Fixed-Bed Reactor: The Performance of Nano-Fe Added Mo/ZSM-5 Catalysts — ***Kaidi Sun***, *Maohong Fan*

9:54 Paper 322g: Effect of Catalyst Composition and Reaction Mechanism Study on Non-Oxidative Methane Conversion into Higher Hydrocarbons — ***Sourabh Mishra,*** *Tuhin Suvra Khan, Sonit Balyan, M. Ali Haider, K. K. Pant*

10:13 Paper 322h: CO_2 Activation by Methane in a Dual-Bed Configuration via Methane Cracking and Iron Oxide Lattice Oxygen Transport: Concept and Materials Development — ***Martin Keller***, *Junichiro Otomo*

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(323) Electrokinetics for Biological Separation and Analysis
Tuesday, Oct 31, 9:00 AM
Hilton, Marquette IV/V/VI/VII

Christopher Palmer, Chair
Aytug Gencoglu, Co-Chair

Sponsored by: 2017 Annual Meeting of the AES Electrophoresis Society

9:00 Paper 323a: Physical Properties of Bioparticles and High-Resolution Separations with Dielectrophoresis — ***Mark A. Hayes***

9:15 Paper 323b: Isomotive Dielectrophoresis-Based Characterization of Chlamydomonas Cells — ***Mohamed Rashed***

9:30 Paper 323c: Characterization of Chemical Affinities and Interactions with Lipid Bilayers Using Electrokinetic Techniques — ***William Penny***, *Christopher Palmer*

9:45 Paper 323d: Numerical Model for Streaming Dielectrophoresis — ***Rucha Natu***, *Monsur Islam, Rodrigo Martinez-Duarte*

10:00 Paper 323e: Automated Selective Cell Manipulation Using Dielectrophoresis — ***Rucha Natu***, *Monsur Islam, Rodrigo Martinez-Duarte*

10:15 Paper 323f: Improving the Understanding of Early-Stage Amyloid Aggregation Using Microchannel Electrophoresis — ***Xavier Redmon***, *Christa N. Hestekin, Melissa A. Moss*

10:30 Paper 323g: Detection of Activated Src in Human Tumor Samples Using 2D SDS Polyacrylamide Gel Electrophoresis — ***Nancy Kendrick***, *Matt Hoelter, Ginny Powers, Andrew Koll, Jon Johansen*

10:45 Paper 323h: Induced Recycle Flow in a Microchannel Using Electroosmosis — ***T. Krishnaveni***, *T. Renganathan, S. Pushpavanam*

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(324) MAC Real Talk: MFF on Academic Career Paths in ChemE (Ticketed Event)
Tuesday, Oct 31, 11:00 AM
MCC, 101F

Belinda Akpa, Chair
Omolola Eniola Adefeso, Co-Chair

Sponsored by: Minority Affairs Committee

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(325) Andreas Acrivos Award for Professional Progress in Chemical Engineering Lecture
Tuesday, Oct 31, 11:15 AM
MCC, Ballroom B

Samir Mitragotri, Chair

Sponsored by: Awards Committee

11:15 Paper 325a: Engineering Amine-Modified Silicates for CO_2 Separations and Catalysis — ***Christopher W. Jones***

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(327) Advances in Chemical Separation Technologies in Nuclear Processes
Tuesday, Oct 31, 12:30 PM
MCC, 200D

John Olson, Chair
Reid Peterson, Co-Chair

Sponsored by: Nuclear Engineering Division

12:30 Paper 327a: Tritium Management Approaches and Their Impacts on Tritium Distribution Within a UNF Reprocessing Plant — ***Robert Jubin***, *Barry Spencer*

12:55 Paper 327b: Effective Removal of Pertechnetate (TcO_4^-), Iodide (I^-) and Iodate (IO_3^-) from Groundwater by Organoclays and Granular Activated Carbon — ***Dien Li***, *Daniel Kaplan, J. C. Seaman, Brian A. Powell, Allison Sams, Steve Heald, Sun Chengjun*

1:20 Paper 327c: Crossflow Filtration Fouling Behavior at Low Solids Concentration — ***Philip P. Schonewill***, *Richard C. Daniel, Carolyn A. Burns, Sabrina D. Hoyle*

1:45 Paper 327d: Performance-Based Simulants for Hanford Radioactive Waste Treatment Process Testing — *Beric Wells,* ***Reid Peterson***, *Richard C. Daniel, Renee Russell*

2:10 Paper 327e: Solids in Hanford's Low-Activity Waste Pretreatment System Feed Tanks and Implications for Design Requirements — ***Jacob Reynolds***, *Stuart T. Arm, Laura Cree*

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(328) Advances in Data Analysis, Information Management, and Intelligent Systems II
Tuesday, Oct 31, 12:30 PM
MCC, 103E

Debangsu Bhattacharyya, Chair
Donald J. Chmielewski, Co-Chair

Sponsored by: Data and Information Systems

12:30 Paper 328a: Variable and Term Selection of Approximations for Data-Driven Optimization — *Sun Hye Kim, Jianyuan Zhai,* ***Fani Boukouvala***

12:51 Paper 328b: Data-Driven Approximation of Feasible Region, Constrained Design of Experiments, and Optimization — ***Ishan Bajaj,*** *M. M. Faruque Hasan*

1:12 Paper 328c: Data-Driven Model Building of Zeolite Adsorption Processes with Uncertainty Quantification and Propagation to Dynamic Simulations of CO2 Adsorption — ***Anca Ostace***, *Debangsu Bhattacharyya, Keenan Kocan, David S. Mebane*

1:33 Paper 328d: Data-Driven Stochastic Robust Optimization: General Modeling Framework and Efficient Computational Algorithm for Handling Labeled Multi-Class Uncertainty Data — ***Chao Ning***, *Fengqi You*

1:54 Paper 328e: Dynamic Canonical Correlation Analysis for the Extraction and Diagnosis of Plant-Wide Oscillations — *Yining Dong,* ***S. Joe Qin***

2:15 Paper 328f: Design of a Supervisory Control System for Inter-Networked Facilities Operation — ***Aaron Driscoll***, *Kyle Cogswell, Matthew Azarian, Aydin K. Sunol, Gita Iranipour*

2:36 Paper 328g: A Graph-Based Modeling and Optimization Framework for Complex Systems — ***Jordan Jalving***, *Yankai Cao, Victor M. Zavala*

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(329) Advances in Distillation Modelling
Tuesday, Oct 31, 12:30 PM
MCC, M100G

Daniel R. Summers, Chair
Andrew W. Sloley, Co-Chair
Clint P. Aichele, Co-Chair

Sponsored by: Distillation and Absorption

12:30 Paper 329a: Tray Pressure Drop Model Development — ***Chao Wang***, *Ken C. McCarley, Tony Cai, Anand Vennavelli*

12:55 Paper 329b: Tomographic Investigation of a Three Phase System in Packed Columns — ***Thomas Linder***, *Wolfgang Arlt*

1:20 Paper 329c: Multiphase Flow Investigations in a Structured Packings Unit — ***Rajesh Singh***, *Janine Galvin, Xin Sun*

1:45 Paper 329d: Improved Control Strategies for Semicontinuous Distillation — ***Pranav Bhaswanth Madabhushi***, *Thomas A. Adams II*

2:10 Paper 329e: Energy-Saving Heterogeneous Extractive Distillation System for the Separation of Close-Boiling Cyclohexane/Cyclohexene Mixture — ***Chun-Cheng Yi***, *Wen-Chi Huang, I-Lung Chien*

2:35 Paper 329f: The Thermodynamics and Separation Process Design for the Ternary System 1,3-Propanediol+ 1,3-Butanediol + 2,3-Butanediol — ***Yanyang Wu***, *Kui Chen, Xiangyang Zhang, Jiawen Zhu*

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(330) Applied Project Management Fundamentals: A Tutorial
Tuesday, Oct 31, 12:30 PM
MCC, L100G

Eldon Larsen, Chair

Sponsored by: Management Division

12:30 Paper 330a: Introduction to the Fundamentals of Project Management — ***Eldon Larsen***

12:50 Paper 330b: The Importance of People in Project Management — ***Eldon Larsen***

1:10 Paper 330c: Communication: A Better Understanding — ***Eldon Larsen***

1:30 Paper 330d: Planning and Conducting Effective Meetings — ***Eldon Larsen***

1:50 Paper 330e: The Importance of Excellent Definition of Project Objectives — ***Eldon Larsen***

2:10 Paper 330f: Overview of Project Planning — ***Eldon Larsen***

2:30 Paper 330g: Application of Basic Project Management Skills to Small-Scale Gas-to-Liquid Projects — ***Lesego M. Moretsele***

(331) Area Plenary: Bionanotechnology I (Invited Talks)
Tuesday, Oct 31, 12:30 PM
MCC, 212A/B

Samantha A. Meenach, Chair
Kathryn A. Whitehead, Co-Chair
Millicent Sullivan, Co-Chair

Sponsored by: Bionanotechnology

12:30 Paper 331a: Multifunctional Polymer Nanoparticles and Fibers by Electrohydrodynamic Co-Jetting — ***Joerg Lahann***

1:20 Paper 331b: Biochemo-Mechanics of Macromolecular Interactions with Lipid Membranes Studied with Microcantilevers — ***Sibani Lisa Biswal***

2:10 Paper 331c: OligoTEA-Based Intracellular Probes and Therapeutics — ***Christopher A. Alabi***

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(332) Area Plenary: Sustainable Biorefineries (Invited Talks)
Tuesday, Oct 31, 12:30 PM
MCC, 101B

Mark Mba Wright, Chair
Vicki S. Thompson, Co-Chair

Sponsored by: Sustainable Biorefineries

12:30 Paper 332a: Development and Demonstration of Advanced Supply Chain Equipment for Harvest, Delivery, and Processing of Herbaceous Biomass — ***Kevin Comer***

1:05 Paper 332b: Feedstock-Driven Operational Challenges Facing Pioneer Biorefineries in the Emerging Biofuel Industry — ***David N. Thompson***, *Damon Hartley, Mohammad Roni, Hongqiang Hu*

1:40 Paper 332c: European Perspective on Feedstocks — ***Anders Jaksland***

2:15 Paper 332d: Perennial Solutions to Annual Problems — ***Emily Heaton***, *Elke Brandes, Mauricio Tejera, Gabe McNunn, Andy VanLoocke, Lisa Schulte*

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(333) Atmospheric Chemistry and Physics II
Tuesday, Oct 31, 12:30 PM
MCC, 102F

Kristina Wagstrom, Chair
Nga Lee Ng, Co-Chair
Shunsuke Nakao, Co-Chair

Sponsored by: Air

12:30 Paper 333a: Contribution of Fugitive Particulate Matter to Airborne Pollution in Arid Areas: A Case Study for an Urbanized Middle Eastern City — ***Hala Hassan***, *Ghadeer Al-Haddad, Nivine Al-Ansari, Prashant Kumar, Konstantinos E. Kakosimos*

12:47 Paper 333b: Study on Regional Air Quality Impact from a Chemical Plant Emergency Shutdown — ***Sijie Ge***, *Sujing Wang, Qiang Xu, Thomas Ho*

1:04 Paper 333c: Source Apportionment and Composition of Fine Particulate Matter in Delhi, India — ***Dongyu S. Wang***, *Sahil Bhandari, Shahzad Gani, Sarah Seraj, Zainab Arub, Gazala Habib, Joshua Apte, Lea Hildebrandt Ruiz*

1:21 Paper 333d: An Improved Hybrid Modeling Framework for Estimation of Human Exposure to Near-Roadway Air Pollution — ***Fatema Parvez***, ***Kristina Wagstrom***

1:38 Paper 333e: Air Filtration of Ultrafine Particles Using PVDF-PEG Hollow Fibers — ***Liang-Yi Wang***, *Yong Wai Fen, Liya E. Yu, Neal Chung*

1:55 Paper 333f: Particle Size Distributions Arising from Vaporized Components of Coal Combustion Fly Ash: A Comparison of Theory and Experiment — *Huimin Liu, Yueming Wang,* ***Jost O. L. Wendt***

2:12 Paper 333g: Cr Speciation in Deliquesced Particulate Matter — ***Mehdi Amouei Torkmahalleh***, *Dinara Konakbayeva, Marios Fyrillas, Altyngul Zinetullina*

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(334) Biomaterial Scaffolds for Tissue Engineering II: Bioactive and Drug-Eluting Materials
Tuesday, Oct 31, 12:30 PM
MCC, 209A/B

Jungwoo Lee, Chair
Kaitlin Bratlie, Co-Chair

Sponsored by: Biomaterials

12:30 Paper 334a: Paper-Based Cell Culture Platforms for Personalized Medicine — ***Gulden Camci-Unal***

12:48 Paper 334b: Growth Factor Delivery from Silk-Extracellular Matrix Composite Sponges for Modulating Congenital Heart Defect Repair — ***Whitney L. Stoppel***, *Elizabeth C. Bender, Luke R. Perreault, Jonathan M. Grasman, Andrea Papait, David L. Kaplan, Lauren D. Black III*

1:06 Paper 334c: Oligodendrocyte Precursor Cell Maturation in a 3D Hydrogel System Through the Incorporation of Drug Delivery Nanoparticles or Topographical Cues — ***Lauren Russell***, *Meghan Pinezich, Kyle Lampe*

1:24 Paper 334d: Resveratrol-Releasing Scaffolds Protect Mice Against Diet-Induced Obesity and Glucose Intolerance — ***Michael Hendley,*** *Prakasam Annamalai, Michael Gower*

1:42 Paper 334e: Silk Fibroin/Xanthan Biopolymeric Composite for Antibiotic-Eluting Wound Dressing — ***Shailendra Singh Shera***, *Rathindra Mohan Banik*

2:00 Paper 334f: Effects of Short-Term Magnetic Stimulation on MSCs Encapsulated in an Injectable, Magneto-Responsive Hydrogel — ***Adedokun Adedoyin***, *Adam Ekenseair*

2:18 Paper 334g: The Incorporation of Retinoic Acid-Like Peptoids onto an Artificial Extracellular Matrix for Increased Differentiation of Human Embryonic Stem Cells into Neural Cells — ***Jesse Roberts***, *German Perez, Shannon L. Servoss*

2:36 Paper 334h: 3D Culture of Trabecular Meshwork Cells — ***Matthew Osmond***

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(335) Biosensors, Biodiagnosis and Bioprocess Monitoring I: Synthetic Biology Approach
Tuesday, Oct 31, 12:30 PM
MCC, 206A/B

Fei Wen, Chair
Kevin J. Cash, Co-Chair

Sponsored by: Bioengineering

12:30 Paper 335a: Direct Quantification of Deubiquitinating Enzyme Activity in Intact Cells Using a Protease-Resistant, Cell-Permeable, Peptide-Based Reporter — *Nora Safabakhsh, Jacob Pettigrew, Gavin Pappas, Ted Gauthier,* ***Adam Melvin***

12:48 Paper 335b: Engineering a Bioluminescence-Based Protein Kinase Reporter for In-Vivo, Longitudinal Studies — ***Evan K. Day***, *Matthew J. Lazzara*

1:06 Paper 335c: Engineering a DNA Polymerase to Become a Calcium-Sensitive Biosensor/Recording Device — ***Bradley W. Biggs***, *Namita Bhan, Alexandra de Paz, Ted Cybulski, Keith E. J. Tyo*

1:24 Paper 335d: Development of Single-Virion Fusion Tool for Assessing Influenza Virus Pandemic Risk — ***Hung-Lun Hsu***, *Gary Whittaker, Susan Daniel*

1:42 Paper 335e: Sort-Seq Approach to Engineering an *E. coli* Formaldehyde-Inducible Promoter — ***Julia R. Rohlhill***, *Nicholas R. Sandoval, Eleftherios T. Papoutsakis*

2:00 Paper 335f: Medium-Throughput Detection of Microbially Produced Serotonin via a GPCR-Based Sensor — *Amy M. Ehrenworth,* ***Pamela Peralta-Yahya***

2:18 Paper 335g: The Role of Nanosensors for Biodiagnostics and Bioprocess Monitoring — ***Michael Strano***

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(336) Breakthroughs in C1 to Chemicals and Processing Engineering
Tuesday, Oct 31, 12:30 PM
MCC, 103A

Zhongmin Liu, Chair
David A. Bell, Co-Chair
Emily Cole, Co-Chair

Sponsored by: Innovations of Green Process Engineering for Sustainable Energy and Environment

12:30 Paper 336a: Methanol to Propylene Process: An Integration of Catalyst Development and Reactor Engineering — ***Mao Ye***, *Peng Tian, Zhongmin Liu*

12:45 Paper 336b: Direct Production of Value-Added Chemicals via Fischer-Tropsch Synthesis — *Liangshu Zhong, Hui Wang, Zhiyong Tang,* ***Yuhan Sun***

1:00 Paper 336c: An Investigation into the Effect of Li and Mn Promotions on the Activity and Selectivities to Olefins and Alcohols of $Co@Co_2C$/Activated Carbon (AC) for Fischer-Tropsch Reaction — ***Yunjie Ding***, *Ziang Zhao, Wei Lu, Hejun Zhu*

1:15 Paper 336d: Direct Production of Gasoline-Range Hydrocarbons from Carbon Dioxide over Iron-Based Multifunctional Catalysts — *Jian Wei,* ***Qingjie Ge***, *Ruwei Yao, Jian Sun*

1:30 Paper 336e: Innovative Syngas Production Catalyst for Utilization of CO_2 (CT-CO_2AR(TM) Catalyst) — ***Takenori Kanda***, *Osamu Hirohata, Tomoyuki Mikuriya, Fuyuki Yagi*

1:45 Paper 336f: Solar Thermochemical Splitting of H_2O and CO_2 Using Nonvolatile Metal Oxides — ***Rahul Bhosale***, *Parag N. Sutar, Gorakshnath Takalkar*

2:00 Paper 336g: Critical Issues in the Development of Commercial Natural Gas to Industrial Chemicals Bioprocesses — ***Bryan Yeh***

2:15 Paper 336h: Process Development for the Production of Bioethylene from Biomass via Gammavalerolactone — ***Aramide Adesina***, *David Lokhat*

2:30 Paper 336i: Direct, Single-Pass Thermocatalytic Upgrading of Biogas and Landfill Gas into Renewable Natural Gas over the Ultra-Low-Loading Ru/γ-Al_2O_3 Catalyst — *Yichen Zhuang,* ***David Simakov***

2:45 Paper 336j: Energy Quality Factor and Exergy Destruction Processes Analysis for a Proposed Polygeneration System — ***GuangJun Meng***, *ZhiPing Zhu, Xuye Jing, Pengfei Dong, Kun Wang*

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(337) Catalysis with Microporous and Mesoporous Materials II
Tuesday, Oct 31, 12:30 PM
MCC, L100A

Bingjun Xu, Chair
Xueyi Zhang, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

12:30 Paper 337a: Mechanistic Implications of Low-Pressure Feeds for Methanol-to-Olefins Conversion on MFI — ***Sukaran S. Arora***, *Aditya Bhan*

12:48 Paper 337b: Catalysis on Microporous Solid Acids: Mechanism and Catalyst Descriptors for the Coupling of Alkenes and Alkanones — ***Michele L. Sarazen***, *Stanley Herrmann, Enrique Iglesia*

1:06 Paper 337c: Structure-Property Relationships for Unidimensional, Large- and Extra-Large-Pore Zeolites Using Alkane Hydrocracking and Hydroisomerization as Probe Reactions — ***Viktor Cybulskis***, *Stacey I. Zones, Tracy Davis, Cong-Yan Chen, Michael W. Deem, Mark E. Davis*

1:24 Paper 337d: Modeling Complex Reactions in Zeolites: Effects of Acid Site Location, Framework, and Reagent Structure on Methanol-to-Hydrocarbon Reactions — *Pavlo Kravchenko, Steven V. Nystrom Jr., Mykela Deluca, Alexander Hoffman,* ***David Hibbitts***

1:42 Paper 337e: Simple Characterization of Solid-Acid Catalysts by Reactive Gas Chromatography — ***Omar A. Abdelrahman***, *Katherine Vinter, Limin Ren, Dandan Xu, Raymond J. Gorte, Michael Tsapatsis, Paul J. Dauenhauer*

2:00 Paper 337f: Understanding Effective Diffusion Length Theory in Nanoscale Zeolites — ***Xiaoduo Qi***, *Vivek Vattipalli, Paul J. Dauenhauer, Wei Fan*

2:18 Paper 337g: 3D-Printed Zeolitic Scaffolds for Selective Transformation of Light Alcohols to Light Olefins — *Xin Li,* ***Ali A. Rownaghi***

2:36 Paper 337h: The Role of Surface Barriers as Dominant Transport Mechanism in Hierarchically Structured Zeolites: Application to the Alkylation of Benzene with Ethylene — ***Sanjeev M. Rao***, *Erisa Saraçi, Roger Glaeser, Marc-Olivier Coppens*

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(338) Catalytic Processing of Fossil and Biorenewable Feedstocks V: Biomass Deconstruction and Oxygenate Processing
Tuesday, Oct 31, 12:30 PM
MCC, L100C

Konstantinos A. Goulas, Chair
Basudeb Saha, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

12:30 Paper 338a: Stabilizing Pd Particles on Nitrogen-Doped Carbon Supports Under Hydrothermal Conditions — ***Jiajie Huo***, *Pu Duan, Hien N. Pham, Abhaya K. Datye, Klaus Schmidt-Rohr, Brent H. Shanks*

12:50 Paper 338b: Reaction Mechanism for the Conversion of γ-Valerolactone (GVL) over an Ru Catalyst — ***Reda Bababrik,*** *Bin Wang, Daniel Resasco*

1:10 Paper 338c: Hydrodeoxygenation of Biomass Derivatives on Metal-Modified Molybdenum Carbides — ***Weiming Wan***, *Jingguang G. Chen*

1:30 Paper 338d: Structure-Activity Relations on γ-Al_2O_3: From Alcohol Dehydration to Alkane Dehydrogenation — ***Pavlo Kostetskyy***, *Giannis Mpourmpakis*

1:50 Paper 338e: Catalytic Non-Aqueous Processing and Hydrogenation of Chitin and Amino-Based Carbohydrates Using Ru Carbene Organometallics Immobilized on Active Hydrotalcites — ***Jacob Heltzel***, *Matthew Finn, Adelina Voutchkova-Kostal*

2:10 Paper 338f: Selective C-C Bond Scission of Biomass-Derived Oxygenates Using Cerium Oxide-Supported Ruthenium Catalyst — ***Tomoo Mizugaki***, *Kohei Uesugi, Kodai Nitta, Zen Maeno, Takato Mitsudome, Koichiro Jitsukawa, Kiyotomi Kaneda*

2:30 Paper 338g: Direct Catalytic Conversion of Cellulose into 2,5-Hexanedione over Pd/C in Formic Acid — ***Jiaguang Zhang***, *Ning Yan*

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(339) Cell Adhesion and Migration II
Tuesday, Oct 31, 12:30 PM
MCC, 208B

Amir M. Farnoud, Chair
Esther W. Gomez, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

12:30 Paper 339a: Fibroblasts Affect Each Other's Directional Decision-Making Process During Chemotaxis in Microfluidic Tissue-Mimicking Mazes — ***Long Quang Pham***, *David Chege, Timothy Dijamco, Sagnik Basuray, Roman Voronov*

12:48 Paper 339b: Nuclear Cytoskeletal Linkages Are Required for Normal Cell Function — ***Qiao Zhang***, *Vincent J. Tocco Jr., Andrew Tamashunas, Yuan Li, Richard Dickinson, Tanmay Lele*

1:06 Paper 339c: Sprouty2 Regulation of Glioblastoma Adhesion and Invasion — ***Nisha G. Sosale***, *Matthew J. Lazzara*

1:24 Paper 339d: The Mechanobiology of Cancer Cell Motility Under Vertical and Lateral Confinement — ***Emily Wisniewski***, *Panagiotis Mistriotis, Robert Law, Alexandros Afthinos, Soontorn Tuntithavornwat, Kaustav Bera, Runchen Zhao, Konstantinos Konstantopoulos*

1:42 Paper 339e: Investigating Changes in Cellular-Based Forces in Monolayers by Tracking Sub-Nuclear Sensors — ***Travis Armiger***, *Marsha Lampi, Cynthia Reinhart-King, Kris Noel Dahl*

2:00 Paper 339f: Compression Affects Short-Time Subdiffusion of Loci and Inclusion Bodies in *E. coli* Cells — ***Shi Yu***, *Marco Gherardi, Marco Cosentino Lagomarsino, Pietro Cicuta, Kevin Dorfman*

2:18 Paper 339g: Investigations of Mechanisms of Force Transduction in Tissues — ***Deborah E. Leckband***

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(340) Chemical Engineering Principles Advancing Medicine II
Tuesday, Oct 31, 12:30 PM
MCC, 202A/B

Thomas A. Zangle, Chair
Charles Reid, Co-Chair

Sponsored by: Chemical Engineers in Medicine

12:30 Paper 340a: Numerical Study of Hemodynamics in the Carotid Artery Before and After Angioplasty with Stenting Using Different Rheological Models — *Carolina A. Sens, Marcela Kotsuka Silva, Henry F. Meier,* ***Jaci Carlo Schramm Camara Bastos***

12:55 Paper 340b: Investigating the Neuroprotective Effects of 5-Hydroxyadamantane-2-One on Middle-Aged Male Rats in an Ischemic Stroke Model — ***Homa Khosravian***, *Min Jung Park, Farida Sohrabji*

1:20 Paper 340c: Blood Damage Predictions Using Computational Fluid Dynamics of Blood Flow Through a Bi-Leaflet Prosthetic Heart Valve — ***Madison James,*** *Edgar A. O'Rear, Dimitrios V. Papavassiliou*

1:45 Paper 340d: Intracellular Mass Transport Estimation Using Quantitative Phase Microscopy — ***Soorya Pradeep***, *Thomas A. Zangle*

2:10 Paper 340e: A Study of Using Synergistic Factors on the Mechanical Properties and Phenotype of Engineered Articular Cartilage Using Atomic Force Microscopy and Immunohistochemistry — *Alia Mallah,* ***Mahmoud Amr***, *Chrystal Quisenberry, Arshan Nazempour, Arda Gozen, Juana Mendenhall, Bernard J. Van Wie,* ***Nehal Abu-Lail***

2:35 Paper 340f: Quantum Molecular Sequencing: Unravelling Genomic Information One Molecule at a Time — ***Prashant Nagpal***

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(341) Chromatographic Separations and SMB
Tuesday, Oct 31, 12:30 PM
MCC, M100E

Yoshiaki Kawajiri, Chair
Arvind Rajendran, Co-Chair

Sponsored by: Adsorption and Ion Exchange

12:30 Paper 341a: An Experimental Validation of the Concurrent Approach for Simultaneous Isotherm Determination and Process Design for Simulated Moving Bed (SMB) System — ***Siwei Guo***, *Yoshiaki Kawajiri*

12:50 Paper 341b: Process Synthesis for Improved Bioseparations Using Multi-Resin Simulated Moving Bed Chromatography — ***Alexander M. Sabol***, *Zachary J. Montoux, Shachit S. Iyer, Jonathan P. Raftery, Ahmed K. Hilaly, M. M. Faruque Hasan, M. Nazmul Karim*

1:10 Paper 341c: Industrial Experience with Model-Based SMB System Design and Optimization: Discretization Scheme and Case Study — ***Wade Martinson***

1:30 Paper 341d: Effects of Operating Parameters, Equipment Parameters, and Material Properties in Ternary Separations in SMB — ***David M. Harvey***, *Nien-Hwa Linda Wang*

1:50 Paper 341e: Simulated Moving-Bed Reactor for Enhancing the Productivities of Equilibrium-Limited Reactions — ***Balamurali Sreedhar***, *Megan E. Donaldson, Timothy C. Frank, Jungmin Oh, Shan Tie, Andreas S. Bommarius, Yoshiaki Kawajiri*

2:10 Paper 341f: Engineering Studies of the Effect of pH and Temperature on the Adsorbent Surface Interaction for the Anion-Exchange Chromatographic Separation — ***James T. Hsu***, ***Gorgi Pavlov***

2:30 Paper 341g: Local Equilibrium Theory Analysis of Chromatographic Peak Shapes in the Presence of Adsorbing Modifiers — ***Arvind Rajendran***

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(342) Combustion Kinetics and Emissions II
Tuesday, Oct 31, 12:30 PM
MCC, L100F

Erdem Sasmaz, Chair
Bihter Padak, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

12:30 Paper 342a: Large Eddy Simulation of Soot Formation in Oxy-Coal Combustion — ***David O. Lignell***, *Alexander J. Josephson, Benjamin Isaac, Kamron Brinkerhoff*

12:52 Paper 342b: Ash Aerosol and Deposition Formation During High-Temperature Oxy-Combustion of Petroleum Coke — ***Yueming Wang***, *Xiaolong Li, Huimin Liu, Jost O. L. Wendt*

1:14 Paper 342c: Mercury Speciation in Oxy-Coal Combustion — ***Nujhat Choudhury***, *Bihter Padak*

1:36 Paper 342d: Improvements in the Efficiency of Staged, Pressurized Oxy-Combustion (SPOC) Process for Power Generation — ***Piyush Verma***, *Akshay Gopan, Zhiwei Yang, Richard Axelbaum*

1:58 Paper 342e: Mediated Oxycombustion with Integrated Uncoupled Oxygen Supply (MOBIUS) — ***Adam Sims***, *Kanchan Mondal*

2:20 Paper 342f: Mobility Size and Effective Density of Carbonaceous Aerosols — ***Georgios A. Kelesidis,*** *Eirini Goudeli, Sotiris E. Pratsinis*

2:42 Paper 342g: Parametric Studies of Soot Formation, Evolution, and Oxidation in Turbulent Jet Flames — ***Victoria B. Lansinger***, *David O. Lignell*

(343) Complex and Networked Chemical and Biochemical Systems
Tuesday, Oct 31, 12:30 PM
MCC, 103F

Mark Styczynski, Chair
Steven M. Abel, Co-Chair
Luis A. Ricardez Sandoval, Co-Chair

Sponsored by:
Applied Mathematics and Numerical Analysis

12:30 Paper 343a: Modeling LPS-Induced TNF-α Production in Macrophages — ***Dongheon Lee***, *Yufang Ding, Arul Jayaraman, Joseph Sangil Kwon*

12:49 Paper 343b: Reaction Network Structure and Flux Analysis for Thin-Film Deposition Processes — ***Hossein Salami***, *Raymond Adomaitis*

1:08 Paper 343c: Hierarchical Modeling and Control of ERK Signaling — *Mohammadreza Yasemi,* ***Yaman Arkun***

1:27 Paper 343d: Parameter Estimation and Sensitivity Analysis in Beer Fermentation Modelling and Dynamic Optimisation — *Alistair D. Rodman,* ***Dimitrios I. Gerogiorgis***

1:46 Paper 343e: Modeling the Influence of the HPA Axis and the Circadian Clock on the Regulation of the Cell Cycle — ***Rohit Rao***, *Kamau Pierre, Eric Hoffman, Ioannis P. Androulakis*

2:05 Paper 343f: Superstructure Optimization of Bio-Refineries Using Metabolic-Network Models — ***Amir Akbari***, *Paul Barton*

2:24 Paper 343g: The Role of Community Structures in Network Control: A Case for the Evolution of Modular Networks in Biology — ***Wentao Tang***, *Prodromos Daoutidis*

2:43 Paper 343h: K-Ath: Towards a Multi-Tissue Kinetic Model of Arabidopsis thaliana — ***Wheaton Schroeder***, *Rajib Saha*

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(344) Continuous Processing Technologies Applied in Drug Product Manufacturing
Tuesday, Oct 31, 12:30 PM
MCC, 204A/B

Mark Barrett, Chair
Joe Hannon, Co-Chair

Sponsored by:
Pharmaceutical Discovery, Development and Manufacturing Forum

12:30 Paper 344a: Assessing the Adequacy of a Sampling Frequency in the Application of PAT to a Continuous Manufacturing Process for Drug Product — ***Salvador García-Muñoz***, *Lukas Barnes, Evan Hetrick, Ian Leavesley, Zhenqi Shi*

12:52 Paper 344b: Continuous Production Technology for Pharmaceutical Semi-Solid and Liquid Formulations: Processability and Influence of Process Parameters on the Product Quality — ***Nils Bostijn***, *Thomas De Beer, Willem Dhondt, Jeroen Van Renterghem, Chris Vervaet*

1:14 Paper 344c: Modeling of Residence Time Distribution of a Continuous Dry-Granulation Tableting Line — ***Michael C. Martinetz***, *Anssi-Pekka Karttunen, Stephan Sacher, Patrick R. Wahl, Ossi Korhonen, Johannes G. Khinast*

1:36 Paper 344d: Robust State Estimation of Feeder and Blender Systems in Continuous Pharmaceutical Manufacturing Systems — ***Jianfeng Liu***, *Qinglin Su, Mariana Moreno, Carl Laird, Zoltan K. Nagy, Gintaras V. Reklaitis*

1:58 Paper 344e: Large-Scale Experimental Comparison of Batch and Continuous Technologies for Pharmaceutical Tablet Manufacturing — ***Kensaku Matsunami***, *Takuya Nagato, Koji Hasegawa, Masahiko Hirao, Hirokazu Sugiyama*

2:20 Paper 344f: A Cost-Benefit Analysis of Continuous Manufacturing Using Discrete Event Simulation — ***Anne Purdy***, *Amy Greer, Palmerly Tom, Ondrej Slama, Pavlo Minayev, Vaclav Belak*

2:42 Paper 344g: Real-Time Monitoring and Control of API Concentration in a Tablet Press for Continuous Manufacturing of Tablets — ***Jin Maeda***, *M. Sebastian Escotet-Espinoza, Ravendra Singh, Marianthi Ierapetritou*

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(345) CO_2 Capture by Adsorption II: Adsorbents
Tuesday, Oct 31, 12:30 PM
MCC, M100F

Joeri Denayer, Chair
Marcus Mello, Co-Chair

Sponsored by:
Adsorption and Ion Exchange

12:30 Paper 345a: Endowing Metal-Organic Frameworks with Scale-Up Production, Hydrophobicity, and Processability for Moisture-Resistant CO_2 Capture — ***Zhigang Hu***, *Dan Zhao*

12:50 Paper 345b: CO_2 Capture in Nitrogen-Doped Porous Carbons Synthesized from Biomass — ***Dipendu Saha***, *Gerassimos Orkoulas*

1:10 Paper 345c: 3D-Printed SAPO-34 Structured Adsorbent for CO_2 Separation — *Sarah Couck, Jasper Lefevere, Vera Meynen, Steven Mullens, Gert Desmet, Gino Baron,* ***Joeri Denayer***

1:30 Paper 345d: Application of Tertiary Amine Containing Hydroxyl Group to Silica-Supported Amine Adsorbent for CO_2 Capture in the Presence of SO_2 — ***Sunbin Jeon***, *Jinseo Min, Ki Bong Lee, Sung Hyun Kim*

1:50 Paper 345e: Identifying Best Core MOFs with Open Mg Sites for CO_2/N_2 Separation Using Computational Tools — ***Hakan Demir***, *Emmanuel Haldoupis, Konstantinos D. Vogiatzis, Evgenii Fetisov, Christopher Cramer, J. Ilja Siepmann, Laura Gagliardi*

2:10 Paper 345f: Oriented Growth of Mg_2(dobpdc) on Honey-Comb Monolith for CO_2 Capture — ***Lalit A. Darunte***, *Krista S. Walton, David S. Sholl, Christopher W. Jones*

2:30 Paper 345g: Spectroscopic Characterization of Humid CO_2 Adsorption on Solid Supported Tertiary Amines — ***Jason Lee***, *Chia-Hsin Chen, Sophia Hayes, Carsten Sievers, Christopher W. Jones*

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(346) CO2 Capture, Utilization, and Disposal: Key to Clean Energy Production I
Tuesday, Oct 31, 12:30 PM
MCC, 200F

Burcu Gurkan, Co-Chair

Sponsored by:
Transport and Energy Processes

12:30 Paper 346a: Hybrid Geothermal Energy Conversion: A Potential Solution for Low-Temperature Geothermal Resources — ***Nagasree Garapati***, *Benjamin Adams, Jeffrey M. Bielicki, Jimmy Randolph, Thomas Kuehn, Martin Saar*

12:55 Paper 346b: On the Origin of Preferred Bicarbonate Production from Carbon Dioxide (CO_2) Capture into Aqueous 2-Amino-2-Methyl-1-Propanol (AMP) — ***Haley Stowe***, *Gyeong Hwang*

1:20 Paper 346c: Evaluating the Performances of Reduction Process in the Solar Thermochemical Two-Step CO_2 Splitting Based on Ceria Redox Reactions — ***Han Zhang***, *Joseph D. Smith*

1:45 Paper 346d: Mass Transfer Studies of Carbon Dioxide Absorption in Sodium Hydroxide in Millichannels — ***Durgadevi A., S. Pushpavanam***

2:10 Paper 346e: Design and Evaluation of Thermodynamic Conditions for an Off-Shore Topside CO_2 Injection System — ***Umer Zahid***

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(347) Developments in Petroleum and Biofuels Refining Technologies II
Tuesday, Oct 31, 12:30 PM
MCC, 200A

Ronald C. Hedden, Chair
Umakanta Jena, Co-Chair
Ian M. Glasgow, Co-Chair

Sponsored by:
Alternate Fuels and New Technology

12:30 Paper 347a: The Effect of New Nanocomposites on Fluidity of Waxy Crude Oil in Low Temperature — ***Huirong Huang***, *Wei Wang, Yanfen Ding, Zeheng Peng, Jing Gong*

12:55 Paper 347b: Co-Processing of Liquid-Phase Pyrolysis Oil and Refinery Intermediates in a Continuous Hydrodeoxygenation Reactor — ***Klara Treusch***, *Nikolaus Schwaiger, Roland Nagl, Berndt Hammerschlag, Julia Ausserleitner, Anna Huber, Peter Pucher, Matthäus Siebenhofer*

1:20 Break

1:45 Paper 347d: Static and Dynamic Catalytic Adsorptive Desulfurization (CADS) of Real Diesel Using Low-Cost TiO_2/Fumed Silica — *Xiaoling Ren, Zewei Liu, Lei Dong,* ***Jing Xiao***

2:10 Paper 347e: [O]-Induced Reactive Adsorptive Desulfurization of Liquid Fuel over Ag_xO@SBA-15 Under Ambient Conditions — *Guang Miao, Liqiong Wu, Ying Wu, Feiyan Ye,* ***Jing Xiao***

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(348) Digital Natives and Digital Tools: Teaching to Millennials with Technology
Tuesday, Oct 31, 12:30 PM
MCC, 205C

Evan K. Wujcik, Co-Chair
Jennifer Pascal, Co-Chair
Amanda Simson, Co-Chair

Sponsored by: Education

12:30 Paper 348a: Quantifying Reading and Online Homework Completion Using an Interactive Material and Energy Balances Textbook — ***Matthew Liberatore***

12:50 Paper 348b: An Open-Access Gate-to-Gate Life-Cycle Assessment for Graduate Researchers — ***Julian Silverman***, *Claudia Bode, Bala Subramaniam*

1:10 Paper 348c: Chemical Engineering Beyond Politics: A Futuristic World Educational System — ***Sohrab Rohani***

1:30 Paper 348d: Enhance Learning Experience by Augmented Reality Tools — ***Konstantinos E. Kakosimos***, *Ghada Salama, Marcelo Castier, Marcin Kozusznik, Saad Moazam, Shaza Shehab*

1:50 Break

2:10 Paper 348f: Introducing Interactive Learning into French University Chemical Engineering Classrooms — ***Veronica Belandria***

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(349) Disability Unity Convocation (Invited Talks)
Tuesday, Oct 31, 12:30 PM
MCC, 101H

Christopher Pope, Chair
Steve Smith, Co-Chair

Sponsored by: Miscellaneous

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(350) Distributed Chemical and Energy Processes for Sustainability
Tuesday, Oct 31, 12:30 PM
MCC, 101D

Paul E. Yelvington, Chair
Carole Read, Co-Chair
Shweta Singh, Co-Chair

Sponsored by: Sustainable Energy

12:30 Paper 350a: Modularized Production of Fuels and Other Value-Added Products from Distributed, Waste or Stranded Feedstocks — ***Robert S. Weber***, *Johnathan E. Holladay, Cynthia Jenks*

12:52 Paper 350b: Novel System for Small-Scale Gasification of Municipal Solid Waste — ***Stephen Cosper,*** *David Waage*

1:14 Paper 350c: Monolithic Catalysts Coated with Hierarchical ZSM-5 for Distributed Fischer-Tropsch Synthesis — ***Chunxiang Zhu***, *David P. Gamliel, Julia A. Valla, George M. Bollas*

1:36 Paper 350d: Valorization of Natural Gas Liquids from Shale Gas — ***Taufik Ridha***, *Yiru Li, Emre Gençer, Jeffrey Miller, Fabio Ribeiro, Rakesh Agrawal*

1:58 Paper 350e: Energy Sustainability Analysis of H_2 Production — ***Carlos E. Gomez Camacho***, *Raffaele Pirone, Bernardo Ruggeri*

2:20 Paper 350f: Chemical Looping–Based Technology for High-Efficiency Production of H_2 from Ammonia (NH_3) — ***Mandar Kathe***, *Kate Clelland, Liang-Shih Fan*

2:42 Paper 350g: Distributed Ammonia Manufacturing — ***Mahdi Malmali***, *Mike Reese, Alon McCormick, Edward L. Cussler*

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(351) Electrocatalysis and Photoelectrocatalysis V: Electrolysis and Solar Fuels
Tuesday, Oct 31, 12:30 PM
MCC, L100D

Adam Holewinski, Chair
N. Aaron Deskins, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

12:30 Paper 351a: Deciphering the Chemical and Physical Mechanisms Active in Elevated-Temperature Photocatalytic Synthesis of Hydrocarbons and Ammonia — ***Siris Laursen***, *Samiksha Poudyal, Morghan Parker*

12:48 Paper 351b: A High-Throughput Computational Screening Approach for Solar Fuels Photoelectrocatalysis — ***Joseph H. Montoya***, *Kristin Persson*

1:06 Paper 351c: Computational Insights into Photo(electro)Chemical Nitrogen Fixation over Titania Catalysts — ***Andrew Medford***, *Benjamin Comer, Marta Hatzell*

1:24 Paper 351d: Engineering the Interface to Improve the Efficiencies of Insulator-Protected Semiconductors for Photoelectrochemical Cells — ***Joseph Quinn***, *Suljo Linic*

1:42 Paper 351e: The Role of Surface-Bound Dihydropyridine Analogs in Pyridine-Catalyzed CO_2 Reduction over Semiconductor Photoelectrodes — ***Thomas P. Senftle***, *Emily A. Carter*

2:00 Paper 351f: Surface Plasmon-Assisted Photoelectrochemical CO_2 Reduction on Well-Defined Nanostructured Silver Electrodes — ***Elizabeth Corson***, *Youngsang Kim, Erin Creel, Fen Qiu, Robert Kostecki, Jeffrey Urban, Bryan D. McCloskey*

2:18 Paper 351g: Artificial Leaf for Carbon Dioxide Photo-Reduction to Fuels — ***Mohammad Asadi***, *Pedram Abbasi, Kibum Kim, Amin Salehi-Khojin*

2:36 Paper 351h: Understanding Photoelectrochemistry on Epitaxial Oxides Through Surface Electronic Structure — ***Kelsey A. Stoerzinger***, *Yingge Du, Scott A. Chambers*

(352) Electrochemical Fundamentals: Faculty Candidate Session
Tuesday, Oct 31, 12:30 PM
MCC, M100C

Maureen H. Tang, Chair
Yushan Yan, Co-Chair
Vijay Ramani, Co-Chair
William E. Mustain, Co-Chair

Sponsored by:
Electrochemical Fundamentals

12:30 Introductory Remarks

12:35 Paper 352a: Rethinking Grid-Level Energy Storage with Minimal Architecture Zinc-Bromine Batteries — ***Kevin Knehr***, *Shaurjo Biswas, Hang Huynh, Daniel Steingart*

2:50 Paper 352b: Highly Energy-Dense Cu-Intercalated Bi-Birnessite/Zn Battery — ***Gautam G. Yadav***

1:05 Paper 352c: Designing Electrolytes for Beyond Li-Ion Batteries Using Coupled High-Throughput Ab-Initio Calculations and MD Simulations — ***Nav Nidhi Rajput***, *Xiaohui Qu, Vijayakumar Murugesan, Karl Mueller, Kristin Persson*

1:20 Paper 352d: Rational Design of Solid-Liquid Interphases for Reactive Metal Batteries — ***Snehashis Choudhury***, *Lynden A. Archer*

1:35 Paper 352e: Molecular Design of Redox-Interfaces: Selective Electrochemical Separations and Beyond — ***Xiao Su***

1:50 Break

2:00 Paper 352j: Atomistic Modeling of Metallic Anodes in Beyond Li-ion Batteries — ***Jeffrey S. Lowe***, *Donald J. Siegel*

2:15 Paper 352g: H_2 Production via Photovoltaic Electrolysis with over 30% Solar-to-Hydrogen Efficiency — ***Jesse D. Benck***, *Linsey C. Seitz, Jieyang Jia, Yijie Huo, Yusi Chen, Jia Wei Desmond Ng, Taner Bilir, James Harris, Thomas F. Jaramillo*

2:30 Paper 352h: Remote-Control Electrodeposition: Design Criteria for Patterning on Substrates Without Direct Electrical Connections — ***Trevor M. Braun***, *Daniel T. Schwartz*

2:45 Paper 352i: Stable Electrochemical Growth in Viscoelastic Flow — ***Shuya Wei***, *Lynden A. Archer*

(353) Environmental Implications of Nanomaterials: Biological Interactions
Tuesday, Oct 31, 12:30 PM
MCC, 210A/B

Cerasela Zoica Dinu, Chair
Alixandra Wagner, Co-Chair
Reem Eldawud, Co-Chair

Sponsored by:
Environmental Aspects, Applications, and Implications of Nanomaterials and Nanotechnology

12:30 Paper 353a: Quantitative Analysis of the Deposited Nanoparticle Dose on Cell Cultures by Optical Absorption Spectroscopy
— Anastasia Spyrogianni, Inge K. Herrmann, Miriam S. Lucas, Jean-Christophe Leroux, ***Georgios A. Sotiriou***

12:49 Paper 353b: Association Rule Mining for Assessing the Relationships Among Biological Responses of Embryonic Zebrafish *— **Muhammad Bilal, Yoram Cohen**, Rong Liu*

1:08 Paper 353c: Dynamic Nanoparticle Restructuring of Lipid Monolayers: Coating Amphiphilicity Trumps Charge *— **Geoffrey D. Bothun**, Nasim Ganji, Iftheker Khan*

1:27 Paper 353d: Examining Effect on Bending Elasticity and Structure of Phospholipid Bilayer Membranes with Embedded Surface-Functionalized Gold Nanoparticles *— **Saptarshi Chakraborty**, Michihiro Nagao, Christopher L. Kitchens*

1:46 Paper 353e: Natural Organic Matter and Bacterial Inoculum Concentration Affect Copper Toxicity to *Escherichia coli* *— **Alex J. Bertuccio,** Joe D. Moore, Robert D. Tilton*

2:05 Paper 353f: Interactions of Engineered Sub-Micron Silica Particles with Cell Membrane Models *— **Ali Asghari Adib**, Alexander L. Kelly, Allan E. David, Amir M. Farnoud*

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(354) Excellence in Graduate Polymer Research (Invited Talks)
Tuesday, Oct 31, 12:30 PM
MCC, 211D

Charles Sing, Chair
Sarah L. Perry, Co-Chair

Sponsored by: Polymers

12:30 Paper 354a: Welcome and Introduction *— **Charles E. Sing**, Sarah L. Perry*

12:45 Paper 354b: Steps Toward Bio-Sourced Packaging: Effect of Composition and Processing on Properties of Co-Polyesters of Polyethylene Terephthalate (PET) with 2,5-Furan Dicarboxylic Acid *— **Anup Joshi**, Maria Coleman*

1:00 Paper 354c: Synthesis and Solution Phase Characterization of Hydroxylated Sulfonated Oligothioetheramides *— **Joseph Brown,** Christopher A. Alabi*

1:15 Paper 354d: Predicting Stable and Metastable Frank-Kasper Phases in Block Polymers Using Self-Consistent Field Theory *— **Akash Arora**, Kyungtae Kim, Morgan W. Schulze, Ronald M. Lewis III, Frank S. Bates, Kevin D. Dorfman*

1:30 Paper 354e: Spatiotemporal Evolution of Structure in Layer-by-Layer Assembled Thin Films Composed of Oppositely Charged Polyelectrolytes *— **Ali Salehi**, Ronald G. Larson*

1:45 Paper 354f: High-Performance Roll-to-Roll Printed PTB7-Th/PCBM Organic Solar Cells *— **Kevin L. Gu**, Xiaodan Gu, Hongping Yan, Zhenan Bao*

2:00 Paper 354g: Pinch-Off Dynamics, Dripping-onto-Substrate (DoS) Rheometry and Printability of Polymeric Complex Fluids *— **Jelena Dinic**, Leidy N. Jimenez, Madeleine Biagoli, Vivek Sharma*

2:15 Paper 354h: Ultra-Fragile "Granular Materials" Designed via a Genetic Algorithm *— **Venkatesh Meenakshisundaram**, Jui-Hsiang Hung, David S. Simmons*

2:30 Paper 354i: Functionalizing Surfaces with Zwitterionic Polymers to Control Cell Adhesion and Direct Neurite Growth *— **Braden Leigh**, Elise Cheng, Corinne Andresen, Marlan Hansen, C. Allan Guymon*

2:45 Paper 354j: Understanding Facilitated Transport of Hydrogen in Polybenzimidazole Containing Palladium Nanoparticles Using an Integrated Experimental and Modeling Approach *— **Lingxiang Zhu**, Deqiang Yin, Shailesh Konda, Mark T. Swihart, Haiqing Lin*

(355) Flow Assurance and Asset Integrity
Tuesday, Oct 31, 12:30 PM
MCC, 200B

Vikram Subramani, Chair

Sponsored by:
Upstream Engineering and Flow Assurance Forum

12:30 Paper 355a: Potential Use of Solid Nanoparticles to Mitigate Hydrate Formation in Water-in-Oil Emulsions in the Presence of Wax *— **Ashwin Kumar Yegya Raman**, Clint P. Aichele*

12:50 Paper 355b: Corrosion Modeling Using Electrochemistry and Computational Fluid Dynamics *— **Kuochen Tsai***

1:10 Paper 355c: Current State-of-the-Art of Gas Hydrates in Flow Assurance *— **Carolyn A. Koh**, Luis E. Zerpa, David T. Wu*

1:30 Paper 355d: Case Study on Microbiological Control Program for Hydraulic Fracturing Operations Using Nitrate-Reducing Bacteria *— **Kiran Gawas,** Chris Rodriguez*

1:50 Break

2:00 Paper 355e: Quantifying Gas Evolution Rates in Complex Hydrocarbon Systems *— **Michael Miranda**, Ashwin Yegya Raman, Alden Daniel, Aniruddha Kelkar, David Lavenson, Sayeed Mohammad, Gene Kouba, Clint P. Aichele*

2:20 Paper 355f: Sand Particle Erosion in Single-Phase and Multiphase Flow *— **Mazdak Parsi**, Mustafa Kara, Partha Sharma*

2:40 Paper 355g: Study on the Pig Motion in Waxy Crude Oil Pipeline During Wax Removing Operation *— **Miao Li,** Jinjun Zhang, Wenwen Liu*

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(356) Fluid-Particle Flow and Reaction Systems II — In Honor of Professor L. S. Fan
Tuesday, Oct 31, 12:30 PM
MCC, 200I

Ah-Hyung Alissa Park, Chair
Raymond Lau, Co-Chair
Zhe Cui, Co-Chair

Sponsored by:
Fluidization and Fluid-Particle Systems

12:30 Paper 356a: Gas-Solid Flows with Tribocharging *— Jari Kolehmainen, Ali Ozel, **Sankaran Sundaresan***

12:55 Paper 356b: DEM Simulations of Flexible and Rigid Fibers for Describing Bulk Flow Behavior *— Yu Guo, **Jennifer Sinclair Curtis***

1:20 Paper 356c: Challenges in CFD Simulation of the Entire Circulating Fluidized Bed (CFB) Loop for Carbon Capture Process *— **Hamid Arastoopour**, Javad Abbasian, Emad Ghadirian, Shahin Zarghami, Emad Abbasi*

1:45 Paper 356d: Discrete Particle Modelling and Analysis of Gas-Solid Flow in Pneumatic Conveying *— Shibo Kuang, **Aibing Yu***

2:10 Paper 356e: Mesoscale Modeling of Multiphase Reactors: Theory and Applications *— **Ning Yang**, Jinghai Li*

2:35 Paper 356f: Reflection from Former Students *— **Ah-Hyung Alissa Park**, Zhe Cui, Raymond Lau, Fanxing Li, Andrew Tong*

2:55 Concluding Remarks *— **A.H.A. Park***

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(357) Functional Nanoparticles
Tuesday, Oct 31, 12:30 PM
MCC, 200J

Christina Tang, Chair
Da Deng, Co-Chair
Georgios A. Sotiriou, Co-Chair
Alexandra Teleki, Co-Chair

Sponsored by: Nanoparticles

12:30 Paper 357a: New Classes of Organic Nanoparticles with Engineered Shape and Functionality: Particles with "Gecko Legs" and Environmentally Benign Antimicrobials *— **Orlin D. Velev***

1:10 Paper 357b: Cellulose Nanocrystal Templates for Transparent Conductive Films *— **Michael J. Bortner**, Kelly Stinson-Bagby, James Owens, Earl J. Foster*

1:30 Paper 357c: Hydrophilic and Hydrophobic Functional Group Interactions on Organic Crystals Coated with SiO2 Nanolayers by Physical Vapor Deposition *— **Anuradha Krishnan**, Elena Rozhkova, Tijana Rajh, Kalyana Pingali*

1:50 Paper 357d: Enzyme-Mimetic Antioxidant Luminescent Nanoparticles for Highly Sensitive Hydrogen Peroxide Biosensing *— Anna Pratsinis, Georgios A. Kelesidis, Frank Krumeich, Jean-Christophe Leroux, **Georgios A. Sotiriou***

2:10 Paper 357e: Physicochemical Characterization of Curcumin-Polymer Nanoparticles and Behavioral Studies of Arthritic Pain in Rats *— **Sonal Mazumder**, Ashish Dewangan, Yamini Perumal, Naresh Pavurala, Kanwaljit Chopra*

2:30 Paper 357f: Polyacid-Functionalized Gold Nanoparticles as an Amyloid-6 Inhibitor Platform *— **Nicholas P. van der Munnik**, Kathleen Mingle, Tao Wei, Jochen Lauterbach, Mark J. Uline, Melissa A. Moss*

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(358) Fundamental Research in Transport Processes
Tuesday, Oct 31, 12:30 PM
MCC, M100D

Jennifer Pascal, Chair
Joel L. Plawsky, Co-Chair

Sponsored by: Transport Processes

12:30 Paper 358a: Searching for Volume Diffusion *— Narendra Singh, T. E. Schwartzentruber, **Edward L. Cussler***

12:45 Paper 358b: Condensation on Highly Superheated Surfaces: Unstable Thin Films in a Wickless Heat Pipe *— **Thao T. T. Nguyen**, Akshay Kundan, Jiaheng Yu, Peter C. Wayner Jr., Joel L. Plawsky*

1:00 Paper 358c: Experimental Investigation of Air Ingress Scenario During Natural Circulation Cooling of a Very Hot Channel *— **Apoorva Rudra**, Sanjoy Banerjee, Masahiro Kawaji*

1:15 Paper 358d: Hydrodynamic Study to Determine Volumetric Mass Transfer Coefficient for Cell Culture Applications *— **Sohail Rasool Lone**, Vimal Kumar, Jeffrey Seay, Derek Englert, Hyun-Tae Hwang*

1:30 Paper 358e: Turbulent Flow of Diutan Biopolymer Solutions and Carbon Nanotube Suspensions in a 4.6 mm ID x 200 L/D Smooth Pipe *— **Preetinder S. Virk***

1:45 Paper 358f: Ionic Transport in Charged Porous Media *— **Jorge Gabitto**, Costas Tsouris*

2:00 Paper 358g: Fluid Dynamics with Superimposed Mass Transfer of Single Bubbles in Reacting Liquids *— **David Merker**, Lutz Böhm, Matthias Kraume*

2:15 Paper 358h: Experimental Temperature and Fluid Flow Measurements in Packed Beds with Magnetic Resonance Imaging *— Matthew Skuntz, James E. Maneval, Dinal Perera, Joseph D. Seymour, **Ryan Anderson***

2:30 Paper 358i: Experimental Study of Gas-Liquid Mass Transfer Enhanced by Bottom Shear Turbulence *— **Tom Lacassagne**, Serge Simoëns, Mahmoud EL Hajem, Jean-Yves Champagne*

2:45 Paper 358j: Influence of Thermophysical Properties of Cryogenic Fluids on Growth and Collapse of Cavitating Bubbles *— **Arpit Mishra**, Rajaram Lakkaraju, Arnab Roy, Parthasarathi Ghosh*

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(359) Fundamentals and Applications for Hazardous Waste Treatment
Tuesday, Oct 31, 12:30 PM
MCC, 102E

Ramesh Chawla, Chair
Robert W. Peters, Co-Chair
Eunsung Kan, Co-Chair
Mohammed Mostafa, Co-Chair

Sponsored by:
Solid and Hazardous Waste

12:30 Paper 359a: Adsorption of Tetracycline Antibiotics in Wastewater onto Biochar-Based Adsorbents *— Yong-Keun Choi, **Eunsung Kan***

12:55 Paper 359b: Reductive Degradation of Co-Contaminant Medium of TCE and Cr(VI) Using Atomized Iron Powder *— **Daniel Attoh**, Aadarsh Shah, Ramesh Chawla*

1:20 Paper 359c: Tritium Distribution and Cycling on Savannah River Site *— **Sandra Cutts**, Robin L. Brigmon, John Seaman, Robert W. Peters*

1:45 Paper 359d: The Mechanism of Engineered Biofilms of Functional Bacteria on Root Surfaces for Organic Contamination Control and Soil Remediation *— **Hongyan Ma***

2:10 Paper 359e: Preparation of Geopolymeric Adsorbent Derived from LD Slag for Removal of Zinc (II) from Waste Water *— **Chayan Sarkar**, Jayanta Kumar Basu, Amar Nath Samanta*

2:35 Paper 359f: Synthesis of "Sea Urchin"-Like Carbon Nanotubes/ Porous Carbon Superstructures Derived from Waste Biomass for Treatment of Various Contaminants *— **Yunjin Yao**, Chao Lian, Guodong Wu, Yi Hu, Fengyu Wei*

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(360) Fundamentals of Interfacial Phenomena I
Tuesday, Oct 31, 12:30 PM
MCC, M100B

David Green, Chair
Marina Tsianou, Co-Chair
Clint P. Aichele, Co-Chair
Bhuvnesh Bharti, Co-Chair
Younjin Min, Co-Chair

Sponsored by: Interfacial Phenomena

12:30 Paper 360a: Interfacial Activity of Silica and Ethyl Cellulose Particles in Fluid-Fluid Interfaces *— **Songcheng Wang**, Yi Zhang, Jiarun Zhou, Ruiyang Zhao, Gregory Benz, Stephane Tcheimou, J. Carson Meredith, Sven H. Behrens*

12:45 Paper 360b: Adhesion of Explosive Particles to Functionalized Surfaces *— **Darby J. Hoss**, Sanjoy Mukherjee, Bryan W. Boudouris, Stephen P. Beaudoin*

1:00 Paper 360c: Interfacial Phase Transitions for Molecular Manufacturing *— **Stoyan Smoukov**, Diana Cholakova, Slavka Tcholakova, Nikolai Denkov, Zhulieta Valkova, Ivan Lesov, Pierre Haas, Raymond E. Goldstein, Jiale Feng, Zahari Vinarov, Tiesheng Wang*

1:15 Paper 360d: Design of New Liquid Crystal-Based Systems with Improved Chemo-Responsiveness Towards the Detection of Nerve Gases *— **Tibor Szilvási**, Nanqi Bao, Nicholas L. Abbott, Manos Mavrikakis*

1:30 Paper 360e: Factors Affecting the Transient Stability of Solid Stabilized Emulsions *— **Ashwin Kumar Yegya Raman**, Michael Miranda, Jarred Kelsey, Jeff White, Clint P. Aichele*

1:45 Paper 360f: Adsorption of Star Polymers to Fluid Interfaces *— Yun-Ru Huang, **Robert D. Tilton***

2:00 Paper 360g: Influence of Order Within Non-Polar Monolayers on Hydrophobic Interactions *— **Nicholas L. Abbott***

2:15 Paper 360h: How Molecular Structure of Surfactants Determines the Dynamics and Viability of Wettability Alteration *— **Soumik Das**, Quoc P. Nguyen, Roger T. Bonnecaze*

2:30 Paper 360i: Chiral Nonlinear Rheology of Phospholipid Monolayers *— **Joseph A. Zasadzinski**, Todd M. Squires, KyuHan Kim, Siyoung Choi*

2:45 Paper 360j: Visualizing Nanoscopic Topography and Patterns in Freely Standing Thin Films *— Yiran Zhang, Subinuer Yilixiati, **Vivek Sharma***

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(361) Graphene 2-D Materials: Synthesis, Functions and Applications II
Tuesday, Oct 31, 12:30 PM
MCC, 213A/B

Vikas Berry, Chair
Placidus B. Amama, Co-Chair

Sponsored by: Carbon Nanomaterials

12:30 Paper 361a: Holey Graphene for Electrochemical Energy Storage *— **Rohit Kanungo,** James G. Radich*

12:50 Paper 361b: Novel 2-D Graphene- 0-D Magnetic Nanoparticle Interfacial Composites *— **Abhilasha Dehankar,** Jinsong Xu, Ethel Perez-Hoyos, Justin Young, Joshua Goldberger, Roland Kawakami, Ezekiel Johnston-Halperin, Jessica O. Winter*

1:10 Paper 361c: Initial Adhesion of Bacterial Cells on Surfaces Functionalized with Graphene Oxide: Insights from AFM-Based Single-Cell Force Spectroscopy *— Jinkai Xue, **Sara BinAhmed**, Zhaoxing Wang, Benjamin Stottrup,**Santiago Romero-Vargas Castrillon***

1:30 Paper 361d: Catalytic CVD Growth of Millimeter-Tall, Single-Wall Carbon Nanotube Carpets Using Industrial Gaseous Waste as a Feedstock *— **Haider Almkhelfe,** Xu Li, Rahul Rao, Placidus B. Amama*

1:50 Paper 361e: Edge Atomic Diffusion in Graphene Nanoribbons and Defect-Engineered Graphene *— **Lin Du**, Ari Gilman, Tam Nguyen, Dimitrios Maroudas*

2:10 Paper 361f: Role of Mo on Single-Walled Carbon Nanotubes Nucleation Catalyzed by MgO-Supported Co *— **Behnaz Rahmani**, Perla B. Balbuena*

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(362) In-Silico Systems Biology II: Health Applications
Tuesday, Oct 31, 12:30 PM
MCC, 207A/B

Rajib Saha, Chair
Mark Brynildsen, Co-Chair
Jason E. Shoemaker, Co-Chair

Sponsored by: Bioengineering

12:30 Paper 362a: Causal Network Modeling of Calcium Wave Propagation in Rat Liver Lobules *— **Aalap Verma**, Anil Antony, Hirenkumar Makadia, Jan Hoek, Babatunde A. Ogunnaike, Rajanikanth Vadigepalli*

12:48 Paper 362b: Characterizing Host Immune Cell and Local Transcriptional Dynamics During Influenza Infection *— **Muying Wang**, Satoshi Fukuyama, Yoshihiro Kawaoka, Jason E. Shoemaker*

1:06 Paper 362c: A Two-State Model-Based Cell Clustering and Network Inference for Single-Cell Gene Expression Data *— **Nan Papili Gao**, Thomas Hartmann, Rudiyanto Gunawan*

1:24 Paper 362d: Maximum-Entropy Approach for Parameter Estimation in Signaling Networks *— **Purushottam Dixit**, Eugenia Lyashenko, Mario Niepel, Dennis Vitkup*

TECHNICAL SESSIONS 2017

1:42 Paper 362e: Computation-Driven Mechanistic Understanding of the Cellular Cost and Regulation of Melanin Production — *Wheaton Schroeder, Jyothi Kumar,* ***Rajib Saha****, Steve Harris*

2:00 Paper 362f: Metabolic Modeling of Interactions Between Pseudomonas aeruginosa and Staphylococcus aureus in Cystic Fibrosis Biofilm Infections — ***Poonam Phalak****, Michael A. Henson, George O'Toole*

2:18 Paper 362g: Hybrid Models Explain Emergent Dynamics in Complex Cell Populations — ***Neda Bagheri***

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(363) Industry Perspectives on Membrane Separations (Invited Talks)
Tuesday, Oct 31, 12:30 PM
MCC, M100H

Nitesh Bhuwania, Co-Chair
Xiaotong Wei, Co-Chair
Dhaval Bhandari, Co-Chair

Sponsored by: Membrane-Based Separations

12:30 Paper 363a: Perspectives on Development of Membranes for Vapor Separation Applications — ***Tim Merkel***

12:55 Paper 363b: Advanced Membranes for Gas Separations: From Dense Films to Asymmetric Membranes — ***Chunqing Liu***

1:20 Paper 363c: Inorganic Membrane Research and Development at ExxonMobil: The Last 25 Years to Today — ***Benjamin A. McCool***

1:45 Paper 363d: Radially Aligned Carbon Nanotube Hollow Fiber Membranes — ***Rob McGinnis***

2:10 Paper 363e: Membranes for Water Purification and Industrial Separations — ***Abhishek Shrivastava***

2:35 Paper 363f: Virus Filtration: The Most Challenging Filtration in Biotech, Process Lessons from a Successful Product Development — ***Gabriel Tkacik***

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(364) Inhomogeneous Polymers
Tuesday, Oct 31, 12:30 PM
MCC, 211B

Pinar Akcora, Chair
Ian Hosein, Co-Chair

Sponsored by: Polymers

12:30 Paper 364a: Engineering Surfaces and Interfaces in Polymer Films with Bottlebrush Polymer Additives — ***Gila Stein****, Rafael Verduzco*

1:00 Paper 364b: Effects of Extensional Flow and Nanoparticle Stabilization on Immiscible Polymer Blend Morphology — ***Matthew S. Thompson****, Sushant Agarwal, Xueyan Song, Rakesh K. Gupta*

1:15 Paper 364c: Non-Isocyanate Polyurethane Thermoplastic Elastomer: Amide-Based Chain Extender Yields Enhanced Nanophase Separation and Properties in Polyhydroxyurethane — ***Goliath Beniah****, David Fortman, William Heath, William Dichtel, John M. Torkelson*

1:30 Paper 364d: Molecular Simulations Study of Solvophobicity Effects on Assembled Structure in Solutions of Amphiphilic Block Copolymers and Nanoparticles — ***Daniel J. Beltran-Villegas****, Arthi Jayaraman*

1:45 Paper 364e: Control Nano/Microstructure Using Photopolymerization-Induced Phase Separation (PhIPS) — ***Erion Hasa****, Julie L. P. Jessop, Jeffrey W. Stansbury, C. Allan Guymon*

2:00 Paper 364f: Spontaneous Self-Assembly and Micellization of Random Copolymers in Organic Solvents — ***Ayse Asatekin***

2:15 Paper 364g: Synthesis and Antibacterial Study of Star-Shaped Poly[2-(dimethylamino)Ethyl Methacrylate]-Based Copolymers with an Inorganic Core — ***Hou Zheng****, Yuji Pu*

2:30 Paper 364h: Understanding Molecular Exchange Kinetics in Polyelectrolyte Complex Micelles — ***Hao Wu****, Jeffrey Ting, Samanvaya Srivastava, Matthew V. Tirrell*

2:45 Paper 364i: Molecular Simulation for the Prediction of Plasticizer Efficiency and Stability in a Polymer Matrix — *Dongyang Li, Kushal Panchal,* ***Li Xi***

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(365) In Honor of Marco Satyro I (Invited Talks)
Tuesday, Oct 31, 12:30 PM
MCC, L100I

Paul M. Mathias, Chair
John M. Shaw, Co-Chair
Walter G. Chapman, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

12:30 Paper 365a: Heavy Oil and Bitumen Complex Viscosity Simulation: Impacts of Phase Behavior on Rheology — ***John M. Shaw****, Sepideh Mortazavi-Manesh, Mildred Becerra*

12:55 Paper 365b: Maxwell and Marco: Thermophysical Property Needs of Rate-Based Process Simulation Tools — ***Ross Taylor***

1:20 Paper 365c: The Expanded Fluid Concept for Transport Property Correlations — ***Harvey W. Yarranton****, **Francisco Ramos-Pallares****, **Shawn D. Taylor***

1:45 Paper 365d: Grid Evaluation of Pure-Compound Properties — ***Vladimir Diky****, Andrei Kazakov, Kenneth Kroenlein*

2:10 Paper 365e: Water Content of Natural Gas Systems in Equilibrium with an Aqueous or a Hydrate Phase: Experimental Measurements and Molecular Modeling — ***Walter G. Chapman****, Wael A. Fouad, Kyoo Song, Kenneth R. Cox*

2:35 Paper 365f: When Experimental and Predicted Data Are in Conflict, What Should We Trust? — ***Ala Bazyleva****, Eugene Paulechka, Vladimir Diky, Joseph W. Magee, Kenneth Kroenlein*

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(366) In Honor of Phil Wankat, the 2016 Recipient of the Warren K. Lewis Award (Invited Talks)
Tuesday, Oct 31, 12:30 PM
MCC, 205D

Richard D. Noble, Co-Chair
C. Stewart Slater, Co-Chair

Sponsored by: Education

12:30 Paper 366a: Chemical Engineering Mobile Apps — ***Jason E. Bara***

12:55 Paper 366b: Process Design: Learning in Chemical Engineering — ***Milo D. Koretsky***

1:20 Paper 366d: Letters from the Editor: Reflections on Phil Wankat — ***Lisa G. Bullard***

1:45 Paper 366e: Blending Teaching, Research and Writing Textbooks — ***Phillip C. Wankat***

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(367) In Honor of Wei-Shou Hu II — 30 Years of Mammalian Cell Culture Engineering for Biologics Manufacturing (Invited Talks)
Tuesday, Oct 31, 12:30 PM
MCC, 208C/D

Emmanuel S. Tzanakakis, Chair
Chetan Goudar, Co-Chair

Sponsored by: Food, Pharmaceutical & Bioengineering Division

12:30 Introductory Remarks

12:35 Paper 367a: Process Analytical Utility of Raman Microspectroscopy for Monitoring Cellular Therapy Manufacturing — ***James M. Piret***

12:55 Paper 367b: Engineering Metabolic Reaction Networks — ***Friedrich Srienc***

1:15 Paper 367c: Stochastic Behavior of Reaction Diffusion Systems: Direct Evaluation of Average Behavior — ***Doraiswami Ramkrishna***

1:35 Intermission

1:45 Paper 367d: From Synthetic Biology to Nano Biotechnology: Rational Antimicrobial Engineering Approaches Towards Combating Drug-Resistant Pathogens — ***Anushree Chatterjee***

2:05 Paper 367e: Cell Culture Engineers' Influence in Cell Therapies — ***Derek Adams***

2:25 Paper 367f: Glycosylation: Trace Metals and Design for Robustness — ***Mugdha Gadgil***

2:45 Comments from Wei-Shou Hu

2:55 Concluding Remarks

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(368) Integrated Process Engineering and Economics Analysis
Tuesday, Oct 31, 12:30 PM
MCC, 103B

Yizu Zhu, Chair
Mike Dou, Co-Chair
Julie N. Renner, Co-Chair

Sponsored by: Innovations of Green Process Engineering for Sustainable Energy and Environment

12:30 Paper 368a: Technical Economic Analysis of an Intensified Integrated Gasification Combined-Cycle Plant Design Featuring Membrane and Adsorptive Reactors — ***Patricia Pichardo****, Vasilios Manousiouthakis, Secgin Karagoz, Theodore Tsotsis, Richard J. Ciora*

12:52 Paper 368b: An Electrochemical Method to Remove Aqueous Sulfide from Swine Manure — ***Yuchuan Wang****, Hongjian Lin, Bo Hu*

1:14 Paper 368c: Pilot-Scale Testing of Electrochemical Removal of Hydrogen Sulfide in Deep-Pit Swine Manure Storage — ***Hongjian Lin****, Yuchuan Wang, Brian Hetchler, Qiyang He, Larry Jacobson, Bo Hu*

1:36 Paper 368d: Economic and Environmental Impact Analyses of Integrated Dehydrogenation and Hydroformylation in Gas-Expanded Liquid Media — ***Dupeng Liu,*** *Raghunath V. Chaudhari, Bala Subramaniam*

1:58 Paper 368e: Bio-Energy with Carbon Capture and Storage (BECCS): Are Inefficient Power Plants a Better Option? — ***Mathilde Fajardy,*** *Niall Mac Dowell*

2:20 Paper 368f: Water Recovery in Coffee Manufacture — ***C. Stewart Slater,*** *Mariano J. Savelski, Christian Wisniewski*

2:42 Paper 368g: Application of Predictive Thermodynamic Models for Industrially Important Systems — ***Yizu Zhu***

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(369) Interfacial and Nonlinear Flows: Particle-Laden Systems
Tuesday, Oct 31, 12:30 PM
Hilton, Marquette I/II/III/VIII/IX

Vivek Sharma, Chair
Pierre Brun, Co-Chair

Sponsored by: Fluid Mechanics

12:30 Paper 369a: Global Strain-Field Mapping of a Carbon Nanotube-Laden Interface Using Digital Image Correlation — ***Sahil R. Vora****, Brice Bognet, Huseini S. Patanwala, Charles Young, Virgile Daux, Anson Ma*

12:45 Paper 369b: Simulations of Transient Dynamics of Dense Suspensions — ***Rui Zhang****, Endao Han, Heinrich Jaeger, Juan de Pablo*

1:00 Paper 369c: Interfacial Rheology of Coexisting Solid and Fluid Monolayers — ***Joesph A. Zasadzinski****, Amit Kumar Sachan, Siyoung Choi, KyuHan Kim, Ka Yee Lee, Luke Hwang, Todd M. Squires*

1:15 Paper 369d: Modulation of Dilatational Rheology with Interfacial Curvature and Phase Morphology — ***Amit Kumar Sachan****, Joesph A. Zasadzinski*

1:30 Paper 369e: Surface Forces, Flows and Fluxes Underlying Nanoridge Formation and Instabilities in Stratifying, Micellar Freestanding Films — *Yiran Zhang,* ***Vivek Sharma***

1:45 Paper 369f: Wrinkling Instabilities in Thin Inhomogenously Stretched Viscous Sheets — ***Siddarth Srinivasan****, Zhiyan Wei, L. Mahadevan*

2:00 Paper 369g: Fluid Instabilities, Density Stratification, and Lee Waves That Result in Growth Limitations and Morphological Instability of Liquid-Crystal Interfaces — ***Jeffrey H. Peterson****, Jeffrey J. Derby*

2:15 Paper 369h: Liquid-Film Coating on Topographically Patterned Rotating Cylinders — ***Weihua Li****, Marcio S. Carvalho, Satish Kumar*

2:30 Paper 369i: Drying of Multicomponent Thin Films on Substrates with Topography — ***Truong Pham****, Xiang Cheng, Satish Kumar*

2:45 Paper 369j: Effect of Elasticity on Stability of Viscoelastic Liquid Curtain — ***Alireza Mohammad Karim****, Wieslaw Suszynski, Lorraine F. Francis, Marcio S. Carvalho*

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(370) K-12 Outreach Activities and Other Broader Impacts
Tuesday, Oct 31, 12:30 PM
MCC, 101I

S. Patrick Walton, Co-Chair
Virginia Davis, Co-Chair

Sponsored by: Education

12:30 Paper 370a: The Women Event: Engaging High School Girls and Their Parents in STEM — *Lakshmi Nathan, Tyler Moeller, Christine Artim, Jessica Akemi Cimada da Silva, Xiang Gu, Lilian C. Johnson, Kevin Kimura, Colleen C. Lawlor, Poornima Padmanabhan, Ghazal Shoorideh, Victoria Sorg, Dana Thornlow,* ***Susan Daniel***

12:55 Paper 370b: Introducing Molecular Gastronomy in K-6 Through a Hands-On Food Spherification and Spaghetti–Fication Experiment — ***Patricia Valenzuela****, **Anju Gupta***

1:20 Paper 370c: Comparison of Web-Based and Lecture-Based Training Approaches to Educate High-School Students with Simulink Modeling Skills — *Kaiyuan Chen, Jianming Geng, Sihan Ling, Nengxin Wang, Muqi Guo,* ***Zuyi (Jacky) Huang***

1:45 Paper 370d: Nanotechnology & Engineering Grand Challenges — ***Virginia Davis****, Joni Lakin, Edward W. Davis*

2:10 Paper 370e: Going Beyond Demonstrations to "Choose Your Own Adventure" Engineering Experiences for Service-Learning K-12 Outreach Opportunities for 3rd-Year Engineering Students and Enhanced Student Engagement for 1st-Year Engineering Students — ***Kristen Wilding****, Bradley C. Bundy*

2:35 Paper 370f: Building Block Air Quality Sensors — ***Anthony Edward Butterfield****, Kerry Kelly, Katrina Le, Colin Pollard, Keenan Lins, Katie Nolan, Piper Stevens, Vaishnathi Thiraviyarajah, Annika Young, Emma Dean*

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(371) Membrane Modeling and Simulation
Tuesday, Oct 31, 12:30 PM
MCC, M100I

Nils Tilton, Co-Chair
Xianghong Qian, Co-Chair
Martin Maldovan, Co-Chair
Dibakar Bhattacharyya, Co-Chair

Sponsored by: Membrane-Based Separations

12:30 Paper 371a: Direct Numerical Simulations of Polarization Phenomena in Direct-Contact Membrane Distillation — ***Jincheng Lou****, Christopher Marks, Johan Vanneste, Christopher Bellona, Steven DeCaluwe, Tzahi Cath, Nils Tilton*

12:45 Paper 371b: Modeling Separations in Mesoporous Membranes Using Lattice-Based and Molecular Simulation Techniques — *Ashutosh Rathi,* ***David M. Ford****, Peter A. Monson*

1:00 Paper 371c: Mass Separation by Metamaterial Membranes — *Juan Manuel Restrepo-Florez,* ***Martin Maldovan***

1:15 Paper 371d: Modeling Bioethanol Enrichment Using Hydrophobic and Hydrophilic Zeolite Membranes — ***Nitish Mittal****, Peng Bai, J. Ilja Siepmann, Prodromos Daoutidis, Michael Tsapatsis*

1:30 Paper 371e: CH_4 and CO_2 Transport Properties Through Nanoporous Graphene and Graphene Oxide Membranes: A Molecular Dynamics Simulation Study — ***Farzin Rahmani****, Amir Khakpay, Sasan Nouranian, Paul Scovazzo*

1:45 Paper 371f: Understanding Water Sorption and Transport in Graphene-Based Membranes from First-Principles-Based Atomistic Modeling — ***Myungsuk Lee****, Gyeong Hwang*

2:00 Paper 371g: Role of Solvent in Structural Reorganization of a Polymer Membrane: An Atomistic Simulation Study — ***Jie Liu****, Jianwen Jiang*

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(372) Micro and Nanofabricated Sensors
Tuesday, Oct 31, 12:30 PM
MCC, M100A

Dongmei (Katie) Li, Chair

Sponsored by: Sensors

12:30 Paper 372a: Development of Highly Sensitive Pico-Calorimetric Sensors Based on Thermoelectric Effect — ***Jinhye Bae****, Haitao Zhang, Joost J. Vlassak*

12:50 Paper 372b: A Micro-Fabricated Electrochemical Gas Sensor for VOCs Detection — ***Pierre-Alexandre Gross****, Sadeghipour Ehsan, Thomas F. Jaramillo, Beth L. Pruitt*

1:10 Paper 372c: Highly Selective, Flame-Made Sensors for Breath Analysis — *Andreas T. Güntner,* ***Sotiris E. Pratsinis***

1:30 Paper 372d: A Drinking Water Sensor for Lead and Other Heavy Metals — *Wen-Chi Lin, Zhongrui Li,* ***Sarah E. Mena****, Mark A. Burns*

1:50 Paper 372e: Real-Time Underwater Detection of Trace Organic Analytes — ***Andrew L. Wagner****, Paul E. Yelvington*

2:10 Paper 372f: Application of Hydrophobic Polymer-Coated TiO2 Nanotube Electrochemical Sensors in Humid Environments — ***Christina Willis,*** *Yalda Saffary, Manoranjan Misra, Swomitra Mohanty*

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(373) Model-Based Integrated Design of Pharmaceutical Drug Substance Processes II
Tuesday, Oct 31, 12:30 PM
MCC, 205A/B

Yuesheng Ye, Chair
Marimuthu Andiappan, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

12:30 Paper 373a: Use of Model Discrimination Method in Drug Substance Process Development — ***Nil Tandogan****, Salvador García-Muñoz, Maitraye Sen, Thomas M. Wilson, Jonas Y. Buser, Stanley P. Kolis, Indrakant V. Borkar, Charles A. Alt*

12:52 Paper 373b: Model-Aided Development for a Mixed Anhydride Formation in a Drug Substance Manufacturing Process — ***Derek Starkey****, Carla Luciani, Kevin P. Cole, Justin Burt, David Mitchell*

1:14 Paper 373c: Design of Efficient Metal Nanocatalysts for Cross-Coupling Reactions Using Finite Difference Time-Domain Simulations — ***Andishaeh Dadgar****, Farshid Mohammadparast, Marimuthu Andiappan*

1:36 Paper 373d: Nonlinear Optimisation of Continuous Artemisinin Crystallisation with Explicit NRTL Model-Based Solubility Prediction — ***Hikaru G. Jolliffe****, Dimitrios I. Gerogiorgis*

1:58 Paper 373e: Moving Horizon-Based Real-Time Optimization and Hybrid Control of Continuous Pharmaceutical Manufacturing Process — ***Ashish Shah***, *Rohit Ramachandran, Ravendra Singh*

2:20 Paper 373f: Multi-Layered Modelling Techniques for the Development of Continuous Manufacturing Processes — ***Philip Donnellan***, *Roderick Jones, Phillip Roche, Brian Glennon*

2:42 Paper 373g: A Refined Non-Random Two-Liquid Segment Activity Coefficient Model for Solubility Modeling — ***Yifan Hao***, *M. R. Islam, Meng Wang, Chau-Chyun Chen*

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(374) Multiscale Systems Engineering II — In Honor of Professor Christodoulos A. Floudas (Invited Talks)
Tuesday, Oct 31, 12:30 PM
MCC, 103C

Efstratios N. Pistikopoulos, Chair
Marianthi Ierapetritou, Co-Chair
Costas D. Maranas, Co-Chair

Sponsored by:
Computing Systems and Technology Division

12:30 Opening Remarks
— ***Marianthi Ierapetritou***

12:35 Paper 374a: Multiscale Optimization Strategies for the Integrated Design, Planning and Scheduling of Process Systems — ***Ignacio E. Grossmann***, *Braulio Brunaud, Cristiana L. Lara, Qi Zhang*

12:58 Paper 374b: Supercritical CO_2 in Production of Biodiesel from Algae: Multiscale Processing — ***Warren D. Seider***, *Cory Silva, Geetanjali Yadav, Lindsay Soh, Julie Zimmerman*

1:21 Paper 374c: On Coarse-Grained and Equation-Free Optimization — ***Ioannis G. Kevrekidis***, *Dmitry Pozharskiy*

1:44 Paper 374d: A Computational ODE Model for the Evaluation of Complement System Activation, Function, and Regulation in Homeostasis and Disease — ***Dimitrios Morikis***, *Nehemiah Zewde*

2:07 Paper 374e: Optimal Distribution of Byproduct Gases, Steam and Power in an Iron and Steel Plant — *Yujiao Zeng*, ***Xin Xiao***, *Jie Li*

2:30 Paper 374f: Global Optimization of Metabolic Reaction Networks — ***Vassily Hatzimanikatis***

2:53 Closing Remarks — ***Stratos Pistikopoulos***

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(375) Nanoelectronic and Photonic Materials I: Nanoscale Applications
Tuesday, Oct 31, 12:30 PM
MCC, 211A

Pabitra Choudhury, Chair

Sponsored by:
Electronics and Photonics

12:30 Paper 375a: Copper-Silver Core-Shell Nanoparticles for Conductive Ink — ***Xiaofeng Dai***

12:41 Paper 375b: Electric Current-Induced Nanoscale Surface Roughness Reduction in Conducting Thin Films — ***Lin Du***, *Dimitrios Maroudas*

12:52 Paper 375c: Unusual Electronic Properties of Template-Directed π-Conjugated Porphyrin and Phosphorene Nanotubes — ***Bryan M. Wong***

1:03 Paper 375d: Complex Pattern Formation from Current-Driven Dynamics of Single-Layer Epitaxial Islands on Crystalline Conducting Substrates — ***Ashish Kumar***, *Dwaipayan Dasgupta, Dimitrios Maroudas*

1:14 Paper 375e: The Infrared and Raman Spectra of Pure-Silica and Aluminosilicate Sodalite — ***Caio Peixoto***, *Amir M. Mofrad, Jack Blumeyer, Liu Jinrui, Karl D. Hammond, Heather K. Hunt*

1:25 Paper 375f: The Effect of Solvent Selection on the Optical Trapping, Manipulation, and Patterning of Nanomaterials — ***Matthew Crane***, *Elena P. Pandres, Patrick Whitham, E. James Davis, Daniel Gamelin, Vincent C. Holmberg, Peter Pauzauskie*

1:36 Paper 375g: Synthesis and Characterization of Electrochemically-Grown Zinc Oxide Nanowires for Use in Rectenna-Based Heat Harvesters — ***Adrian Haley***, *Shendu Yang, Patrick J. Pinhero*

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(376) Nanomaterials for Hydrogen Production and Fuel Cells
Tuesday, Oct 31, 12:30 PM
MCC, 200G

Yong L. Joo, Chair
Jinwoo Lee, Co-Chair
Doh Change Lee, Co-Chair

Sponsored by:
Nanomaterials for Applications in Energy and Biology

12:30 Paper 376a: Impact of Ionomer Resistance in Nanofiber-Nanoparticle Electrodes for Ultra-Low-Platinum Fuel Cells — ***Monica Hwang***, *Yossef A. Elabd*

12:48 Paper 376b: Plant Cell Wall–Inspired Nanoscale Materials for Renewable Energy Applications — ***Shudipto Konika Dishari***

1:06 Paper 376c: Engineering High-Performance and Durable PGM-Free Electro-Catalysts for Oxygen Evolution Reaction in PEM Water Electrolysis — ***Shrinath Ghadge***, *Oleg Velikokhatnyi, Moni Kanchan Datta, Prasad P. Patel, Prashant Kumta*

1:24 Paper 376d: Electroactivity and Stability Analysis of Nickel-Oxide Nanoclusters Deposited on Graphene with Ball Milling and Microwave-Assisted Deposition for Glucose Sensing and Fuel Cells — ***Matthew DeCuir***, *Ram B. Gupta*

1:42 Paper 376e: A Combined High-Throughput Computing and Machine Learning Study Reveals Hydrogen Storage Performance Ceilings of Metal-Organic Frameworks — ***Alauddin Ahmed***, *Donald J. Siegel*

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(377) New Developments in Computational Catalysis II
Tuesday, Oct 31, 12:30 PM
MCC, L100E

Heather J. Kulik, Chair
Eric Walker, Co-Chair
Shaama Mallikarjun Sharada, Co-Chair
Bin Liu, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

12:30 Paper 377a: Simulating Solvent Effects in Catalytic Systems — ***Matthew Neurock***, *Peng Bai, Chotitath Sanpitaksere*

1:01 Paper 377b: Electronic Excitations in Thermal Heterogeneous Catalysis — ***Matthew M. Montemore***, *Robert Hoyt, Grigory Kolesov, Efthimios Kaxiras*

1:18 Paper 377c: Large-Scale Nonadiabatic Molecular Dynamics Enabled by Machine Learning — ***Jiamin Wang***, *Hongliang Xin*

1:35 Paper 377d: Modeling of Segregation on Au-Pd (111) Surfaces with Monte Carlo Simulations and Neural Network Atomic Potentials — ***Jacob R. Boes***, *John R. Kitchin*

1:52 Paper 377e: Accelerating Electronic Structure Calculations with Machine Learning — ***Andrew A. Peterson***, *Alireza Khorshidi*

2:09 Paper 377f: A Data-Driven In-Silico Research Paradigm for the Rational Design of Catalyst Systems and the Exploration of Chemical Space — ***Johannes Hachmann***

2:26 Paper 377g: Overcoming the Compromise Between Accuracy and Efficiency in Modelling Catalytic Kinetics — ***Miguel Pineda***, *Michail Stamatakis*

2:43 Paper 377h: CO Adsorption on Platinum and Cobalt: Site Preference and Coverage Effects — ***G. T. Kasun Kalhara Gunasooriya***, *Mark Saeys*

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(378) Particle Breakage and Comminution Processes
Tuesday, Oct 31, 12:30 PM
MCC, 200H

Priscilla J. Hill, Chair
Ecevit Bilgili, Co-Chair

Sponsored by:
Particle Production and Characterization

12:30 Paper 378a: Grindability of Torrefied Wood Pellets — ***Maryam Manouchehrinejad***, *Sudhagar Mani*

12:49 Paper 378b: Effect of Media Shape on Impact Breakage of a Bed of Silica Sand Particles: An Attainable Region Approach — ***Nkosikhona Hlabangana***, *Nonhlanhla G. Mguni, Gwiranai Danha*

1:08 Paper 378c: DEM-PBM Modelling of the Milling Process of Pharmaceutical Ribbons — ***Chuan-Yu Wu***

1:27 Paper 378d: Modeling of Particle Breakage and Dispersion in a Slurry Fischer-Tropsch Reactor — ***Deekshitha Adapa***, *Aruna C. M., Udaya Bhaskar Reddy Ragula*

1:46 Paper 378e: Perspectives on Rotor Stator Wet Milling: Scaledown, Scaleup, Operations and Applications — ***Ivan Lee***, *Eric Sirota*

2:05 Paper 378f: Crystal Wet Milling and Particle Attrition in High-Shear Mixers — ***Kanan Ghaderzadeh***, *Richard V. Calabrese*

2:24 Paper 378g: An Investigation into the Performance of an Industrial-Scale Roll Mill — ***Karl Jacob***, *James F. Koch, Ben Freireich, Madhusudhan Kodam*

2:43 Paper 378h: A Novel Multiscale Modeling Approach for Simulating the Evolution of Particle Size During Dry Milling — ***Ecevit Bilgili***, *Maxx Capece, Rajesh N. Dave*

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(379) Particle Formation and Crystallization Processes from Liquids, Slurries, and Emulsions
Tuesday, Oct 31, 12:30 PM
MCC, M100J

Lotfi Derdour, Chair
Jason Sweeney, Co-Chair

Sponsored by:
Crystallization and Evaporation

12:30 Welcoming Remarks

12:35 Paper 379a: Surface Dynamics of Calcium Oxalate Monohydrate Crystallization: Elucidating Mechanisms of Growth Inhibition — ***Bryan Alamani***, *Doyoung Kim, Ricardo Sosa, Jeffrey D. Rimer*

12:55 Paper 379b: Use of the Constant Composition Method to Evaluate the Nucleation and Growth Kinetics of Calcium Biominerals — *Gopichand Mallam, Christine Moore*, ***Marina Tsianou***

1:15 Paper 379c: Polymorphism of D-Mannitol: Nucleation and Crystal Growth of the Metastable Polymorphs — ***Weiyi Su***, *Chunli Li, Honghai Wang, Jing Fang*

1:35 Paper 379d: Solution-Mediated Polymorphic Transformation of Cefaclor: Insights into the Interaction Between Polymorph Surfaces — ***Chang Wang***, *Xia Zhang, Yaohui Huang, Qiuxiang Yin*

1:55 Paper 379e: A Case of a Twisty Route to First Crystals — ***Lotfi Derdour***

2:15 Concluding Remarks

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(380) Particulate and Multiphase Flows: Colloidal and Granular Systems
Tuesday, Oct 31, 12:30 PM
Hilton, Conrad D

Lilian Hsiao, Chair
Ali Mohraz, Co-Chair

Sponsored by: Fluid Mechanics

12:30 Paper 380a: Flow, Arrest and Yielding in Dense Colloidal Suspensions: Glasses vs. Gels — ***Chinedum O. Osuji***

1:00 Paper 380b: Modeling a Hydrodynamic Instability in Freely Settling Colloidal Gels — ***Zsigmond Varga***, *Jennifer L. Hofmann, James Swan*

1:15 Paper 380c: Effects of Attractive Interparticle Interactions on Normal Stresses and Shear-Induced Migration of Colloids — *Nayoung Park*, ***Jacinta C. Conrad***

1:30 Paper 380d: Connecting Bidisperse and Polydisperse Suspension Rheology — ***Sidhant Pednekar***, *Jaehun Chun, Jeffrey F. Morris*

1:45 Paper 380e: The Steric Effect of a Solid Boundary on the Orientation Distribution of a Dilute Suspension of Rigid Rod-Like Particles Under Shear Flow — *Saman Monjezi, James Jones, Shawn Oettle*, ***Joontaek Park***

2:00 Paper 380f: Particle Crystallinity in Automated Langmuir-Blodgett Deposition: Effect of Speed and Concentration — ***James F. Gilchrist***, *Kedar Joshi, Zhiqiao Zeng, Xue Li*

2:15 Paper 380g: A Hybrid Lattice Boltzmann-Random Walk Method for Multiphase Heat Transfer — ***Aaron Lattanzi***, *Xiaolong Yin, Christine Hrenya*

2:30 Paper 380h: Separation by Design: Towards Simulation-Guided Engineering of Coiled Channels for Precise Particle Separation — ***Jakob D. Redlinger-Pohn,*** *Federico Municchi, Stefan Radl*

2:45 Paper 380i: Simulations of Particle-Laden Flows in Microchannels — *Wouter Van Aeken, Khurram Shahzad, Tom Van Gerven*, ***Simon Kuhn***

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(381) Polymer Networks and Gels
Tuesday, Oct 31, 12:30 PM
MCC, 211C

Eric W. Cochran, Chair
Mingjiang Zhong, Co-Chair

Sponsored by: Polymers

12:30 Paper 381a: The Thiol-Thioester Exchange in Network and Linear Polymers — ***Christopher N. Bowman***, *Brady Worrell, Matthew K. McBride, Gayla Berg, Chen Wang*

1:00 Paper 381b: Nacre-Inspired Composite Gels for Biomedical Applications — ***Ayomi S. Perera***, *Richard Jackson, Mark Miodownik, Marc-Olivier Coppens*

1:15 Paper 381c: Dual-Cure Polymer Networks with Improved Imprintability: Engineering a First-Stage Supramolecular Network — ***J. Taylor Goodrich***, *Hannah Coley, Lewis Cox, Christopher N. Bowman*

1:30 Paper 381d: High-Viscosity Polymer Gels Derived from Block Copolymer Nanocomposites — ***Sri Harsha Kalluru***, *Eric W. Cochran*

1:45 Paper 381e: Quantifying Topology, Gelation and Elasticity of Polymer Networks — ***Rui Wang***, *Bradley D. Olsen*

2:00 Paper 381f: Self-Assembly and Mechanical Properties of Di-FMOC-L-Lysine-Containing Molecular Gels — *Seyed Meysam Hashemnejad, Md. Masrul Huda, Neeraj Rai*, ***Santanu Kundu***

2:15 Paper 381g: Thermoresponsive Sol-Gel Transitions of PEG-Based Nanocomposite Hydrogels Controlled by Molecular Weights of Block Copolymers and Solute Concentrations — ***Tomoki Maeda***, *Midori Kitagawa, Keishi Tanimoto, Makoto Miyazaki, Koji Nagahama, Atsushi Hotta*

2:30 Paper 381h: Evaluating Reprocessability of Polymer Networks: Flory-Stockmayer Analysis — ***Lingqiao Li***, *Xi Chen, Kailong Jin, John M. Torkelson*

2:45 Paper 381i: Molecularly Templated Reaction for Forming Poly(dimethyl siloxane)/Graphene Oxide Composite Elastomers — ***Heonjoo Ha***, *KiRyong Ha, Christopher J. Ellison*

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(382) Process Intensification by Process Integration
Tuesday, Oct 31, 12:30 PM
MCC, 101E

Andrei Merenov, Chair
Hannsjörg Freund, Co-Chair

Sponsored by:
Process Intensification & Microprocess Engineering

12:30 Paper 382a: Towards Biorefinery Process Integration in Oil Refineries — ***Harvey Arellano-Garcia***, *Elham Ketabchi, Tomás Ramirez-Reina*

12:49 Paper 382b: Process Intensification in the Synthesis of Tributyl Citrate: Pilot-Scale Validation — ***Miguel Santaella***, *Alvaro Orjuela, Felipe Martinez, Gerardo Rodriguez*

1:08 Paper 382c: Process Intensification in Multicomponent Distillation — ***Zheyu Jiang***, *Mohit Tawarmalani, Rakesh Agrawal*

1:27 Paper 382d: Analysis of Key Metrics in the Use of Oxidative Dehydrogenation for the Production of Ethylene from Shale Gas Ethane — ***Anne Gaffney***, *Gennaro J. Maffia*

1:46 Paper 382e: Continuous Manufacturing as an Enabler for Intensified Process Design and an Integrated Control Strategy in Pharmaceutical Synthesis — ***Brandon Reizman***, *Molly Hess, Kevin P. Cole, Justin Burt, Martin D. Johnson, Todd D. Maloney, David Mitchell*

2:05 Paper 382f: A Systematic Method for Chemical and Biochemical Sustainable Process Synthesis, Design and Intensification — ***Nipun Garg***, *John M. Woodley, Rafiqul Gani*

2:24 Paper 382g: Strategies for Process and Size Selection of Natural Gas Liquefaction Processes: Specific Profit Portfolio Approach by Cost-Based Optimization — ***Inkyu Lee***, *Il Moon*

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(383) Process Modeling and Identification
Tuesday, Oct 31, 12:30 PM
MCC, 103D

Daniel Chen, Chair
Q. Peter He, Co-Chair

Sponsored by:
Systems and Process Control

12:30 Paper 383a: Virtual Metrology as a Big-Data Solution to Semiconductor Manufacturing — ***Kerul Suthar***, *Devarshi Shah, Q. Peter He*

12:47 Paper 383b: Enabling Discovery and Integration of Process Models and Data Using Ontology in the Domain of Biorefining — ***Linsey Koo***, *Edlira Kalemi, Franjo Cecelja*

1:04 Paper 383c: Multivariable Adaptive Subspace Identification of Blood Glucose Concentration Dynamics for People with Type 1 Diabetes Mellitus — ***Iman Hajizadeh***, *Mudassir Rashid, Sediqeh Samadi, Mert Sevil, Nicole Frantz, Jianyuan Feng, Caterina Lazaro, Zacharie Maloney, Rachel Brandt, Xia Yu, Kamuran Turksoy, Elizabeth Littlejohn, Ali Cinar*

1:21 Paper 383d: Model Reduction and Approximation for Simultaneous Design, Control, and Scheduling — ***Justin Katz***, *Baris Burnak, Nikolaos A. Diangelakis, Efstratios N. Pistikopoulos*

1:38 Paper 383e: Handling Delayed and Irregular Measurements in Batch Subspace Model Identification Framework — ***Abhinav Garg***, *Prashant Mhaskar*

1:55 Paper 383f: Design of Experiments for Identification of a Model That Is Suitable for Use in Control System — ***Shobhit Misra***, *Michael Nikolaou*

2:12 Paper 383g: How Does a Control Room Operator Identify the Process? Insights Using a Cognitive Engineering Approach — *Laya Das, Babji Srinivasan*, ***Rajagopalan Srinivasan***

TECHNICAL SESSIONS 2017

2:29 Paper 383h: Predictive Control of Lake Levels and Estimation of Stream Flows for the Adaptive Management Complex Natural Watersheds, Part 1: Estimation — ***Jeffrey C. Kantor***

2:46 Paper 383i: Predictive Control of Lake Levels and Estimation of Stream Flows for the Adaptive Management Complex Natural Watersheds, Part 2: Economic Model Predictive Control — ***Jeffrey C. Kantor***

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(384) Process Research & Innovation for Improved Process Efficiency
Tuesday, Oct 31, 12:30 PM
MCC, 102B

Tom Xu, Chair
Tom Enright, Co-Chair

Sponsored by:
Process Research and Innovation

12:30 Paper 384a: Multi-Objective Optimization of Crude Distillation Unit, Vacuum Distillation Unit and Hydrocracking Reactor in Diesel Production Process to Maximize Profitability and Reduce Greenhouse Gases Using NSPSO and NSGA-II Bioinspired Techniques — ***Camilo Monroy-Peña***, ***Johana Orjuela***

12:55 Paper 384b: Optimization of Series and Parallel Flow Configurations of Vapor Absorption Chiller — ***Muhammad Zaman***, *Muhammad Usman Ghani*

1:20 Paper 384c: Modelling and Optimization Approaches to Enhance the Efficiency of Heat Recovery Steam Generators: A Case Study in Industrial Combined-Cycle Power Plant — *Parag Shankar Patil, Babji Srinivasan,* ***Rajagopalan Srinivasan***

1:45 Paper 384d: Development of a Computational Fluid Dynamic Modelling Concept for the RecoDust Process — ***Franz Edler***, *Christoph Spijker, Harald Raupenstrauch, Johannes Rieger, Bernhard Geier, Wolfgang Reiter*

2:10 Paper 384e: Dynamic Simulation and Optimization for Gas-Expanded Liquid Phase of Ethylene Oxide Production with Free Carbon Dioxide Emission — ***Mhd A. Abou Shama***, *Qiang Xu*

(385) Reaction Chemistry and Engineering II
Tuesday, Oct 31, 12:30 PM
MCC, L100B

Saif A. Khan, Chair
Klavs F. Jensen, Co-Chair
Milad Abolhasani, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

12:30 Paper 385a: Revealing Cellulose Pyrolysis Initiation Kinetics via Novel Millisecond Pulse Reactor System — *Cheng Zhu, Christoph Krumm,* ***Gregory G. Facas***, *Matthew Neurock, Paul J. Dauenhauer*

12:52 Paper 385b: Role of Co-ZSM-5 in the Low-Temperature Aerobic Selective Oxidation of Neat Ethylbenzene — ***Anyang Peng***, *Linping Qian, Ruiyi Yan, Mayfair C. Kung, Harold H. Kung*

1:14 Paper 385c: Oxidation of Dibenzothiophene in Diesel by In-Situ Generation of Hydrogen Peroxide in a Trickle-Bed Electrochemical Reactor — ***Ghassan Abdullah***, *Yangchuan Xing*

1:36 Paper 385d: Materials Design Strategies for Performing 'Unmixed Reactions' Using Non-Stoichiometric Solids as Oxygen Carriers — ***Ian S. Metcalfe***

1:58 Paper 385e: Fundamentals of the Removal of Sulfur Compounds from Gaseous Streams via Reactive Sorption with Copper Oxide — ***Sara Azzam***, *Dante Simonetti*

2:20 Paper 385f: The Mechanism and Kinetics of Magnesium Oxide Carbothermic Reduction — ***Adrian Coray***, *Zoran R. Jovanovic, Aldo Steinfeld*

2:42 Paper 385g: Enhancing the Rate of Magnesium Oxide Carbothermal Reduction by Catalysis, Mechanical Milling, and Vacuum — ***Boris Chubukov***, *Aaron W. Palumbo, Scott Rowe, Mark Wallace, Alan W. Weimer*

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(386) Separation Processes in Biorefineries
Tuesday, Oct 31, 12:30 PM
MCC, 200E

Bandaru V. Ramarao, Chair
Shri Ramaswamy, Co-Chair

Sponsored by:
Biorefinery Technologies for Forest-Based Lignocellulosic Biomass

12:30 Paper 386a: Separation of Anhydrosugars and Phenolic Species in a Fast-Pyrolysis Aqueous Product Stream Using Resin Adsorbents and Simulated-Moving-Bed Technology — ***John Stanford***, *Patrick H. Hall, Marjorie Rover, Ryan Smith, Robert Brown*

12:50 Paper 386b: Use of Novel Reactor-Separator Combination (Membrane BioReactor) for the Enzymatic Hydrolysis of Waste Fines and Fiber Rejects from Recycled Linerboard Paper Mills — ***Surya Jampana***

1:10 Paper 386c: Evolving Topochemistry of Acer saccharum Chips During Pretreatment Determined by Confocal Raman Microscopy — ***Christopher Thomas***, *Bandaru V. Ramarao, Shri Ramaswamy, Feng Xu*

1:30 Paper 386d: Synthesis of Silver Nanoparticles Using Extracellular Polymeric Substances from Cosmarium sp. Using Microwave — ***Adarsh Bafana***, *Shishir V. Kumar, Prasad P. Pawar, Ashiqur Rahman, Si A. Dahoumane, Clayton S. Jeffryes*

1:50 Paper 386e: First Proof of Supported Hydrophobic Deep Eutectic Solvent Liquids Membranes for the Removal of Furfural and 5-(hydroxymethyl)Furfural from an Aqueous Environment — ***Carin Dietz***, *Maaike C. Kroon, M. van Sint Annaland, Fausto Gallucci*

2:10 Paper 386f: Use of Competitive Adsorption with 2,5-Dimethylfuran for the Inhibition of Isomerization and Dimerization Products — ***Katherine P. Vinter***, *Paul J. Dauenhauer*

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(387) Separation Process Improvements for Sustainability
Tuesday, Oct 31, 12:30 PM
MCC, 101C

Lindsay Soh, Chair
Jeffrey McCutcheon, Co-Chair

Sponsored by: General

12:30 Paper 387a: Desorption of Gases from Ionic Liquids Using an Applied Electric Field — ***William J. R. Gilbert***, *Mark B. Shiflett*

12:52 Paper 387b: Application of GAMS in the Validation of an Experiment-Based Full-Factorial Dual-Objective Adsorption System for the Analysis of Process Variable Effects — ***Mutiu Amosa***, *Thokozani Majozi*

1:14 Paper 387c: Tempo-Oxidized Cellulosic Membranes for Low Fouling Applications — ***Jamie A. Hestekin***, *John Moore, Peter Crooks, Narsimha Penthala*

1:36 Paper 387d: Techno-Economic Analysis of Polymeric Membrane Systems for Post-Combustion Carbon Capture — ***Yang Han***, *W. S. Winston Ho*

1:58 Paper 387e: An Outlook on Hydrogen Production from Bio-Ethanol Reforming Reactions by Membrane Reactor Technology: Opportunities and Challenges — ***Simona Liguori***, *Jennifer Wilcox*

2:20 Paper 387f: FO Separations with High-Performance TFC Membranes and Novel Draw Solutes — ***Yan Wang***, *Liang Shen, Qingwu Long, Shu Xiong, Xuan Zhang, Jiaqi Huang*

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(388) Structure in the Design of Sustainable Processes and Supply Chains
Tuesday, Oct 31, 12:30 PM
MCC, 102A

Ferenc Friedler, Chair
Heriberto Cabezas, Co-Chair

Sponsored by: Fundamentals

12:30 Introductory Remarks

12:33 Paper 388a: The Last Quarter Century of Methods and Software for Algorithmic Process Synthesis — ***Botond Bertok***, *Zoltán Süle, Ferenc Friedler*

12:57 Paper 388b: Near-Term and Sustainable Carbon Dioxide Removal: Is Bio-Energy with Carbon Capture and Storage (BECCS) the Right Answer? — ***Mathilde Fajardy***, *Niall Mac Dowell*

1:21 Paper 388c: A Physical Input-Output Model for the Food-Energy-Water (FEW) Nexus in Indiana — ***Elizabeth Wachs***, *Shweta Singh*

1:45 Paper 388d: Synthesis of Sustainable Systems Using the Novel Sustainability over Sets (SOS) Concept — ***Vasilios Manousiouthakis***, *Masih Jorat*

2:09 Paper 388e: Interventions for Reducing Energy Impacts of Water Embodied in Domestic Food Trade: A Network Perspective — ***Nemi Vora***, *Vikas Khanna*

2:33 Paper 388f: A General Framework for Process and Utility Networks Synthesis — ***Salih E. Demirel***, *Jianping Li, M. M. Faruque Hasan*

2:57 Concluding Remarks

(389) Symposium on Solar Power and Chemical Systems in Honor of Prof. Edward A. Fletcher II
Tuesday, Oct 31, 12:30 PM
MCC, 201A/B

Nick AuYeung, Chair
Mahesh Venkataraman, Co-Chair
Christopher L. Muhich, Co-Chair

Sponsored by:
Symposium on Solar Power and Chemical Systems in Honor of Prof. Edward A. Fletcher

12:30 Paper 389a: Keynote — Two-Step Solarthermal Water Splitting: The Path Forward — ***Alan W. Weimer***

1:00 Paper 389b: Syngas Production via Solar Chemical-Looping Reformation of Methane in a Fixed-Bed Reactor — ***Jesse R. Fosheim***, *Brandon J. Hathaway, Jane H. Davidson*

1:20 Paper 389c: Solar Gasification in a Molten Salt Reactor for Continuous Production of Syngas — ***Brandon Hathaway***, *Nathaniel Lewin, Jane H. Davidson*

1:40 Paper 780f: An Evaluation of Feedback and Model Predictive Control for the Rejection of Weather Transients in Renewable High-Temperature Solar Thermal Chemical Processing on a Novel Hybrid Solar-Electric Reactor — ***Scott Rowe***, *Illias Hischier, Boris Chubukov, Mark Wallace, David E. Clough, Alan W. Weimer*

2:00 Paper 389e: Solar Hybrid Photo-Thermochemical Sulfur-Ammonia Water-Splitting Cycle: Photocatalyst, Thermodynamics and Plant Analysis — ***Konstantinos E. Kakosimos***, *Agni E. Kalyva, Ekaterini Vagia, Abdur Rahman Shazed, Rashid Al-Heidous, Nazim Muradov, Ali T-Raissi, Arun Srinivasa*

2:20 Paper 389f: On the Potential for Enhancement of Solar Thermochemical Synthesis Processes by Nonequilibrium Plasma — *Dassou Nagassou, Sina Mohsenian, Rasool Elahi,* ***Juan P. Trelles***

2:40 Paper 389g: Direct Two-Step Solar Metallothermic and Electrolytic Production of Rare Earth Elements from Oxides — *Mahesh Venkataraman,* ***Peter Kreider***, *Wojciech Lipinski*

(390) Synthetic Biology Applications II: Microbial Biosynthesis
Tuesday, Oct 31, 12:30 PM
MCC, 208A

Nanette R. Boyle, Chair
Peng Xu, Co-Chair

Sponsored by: Bioengineering

12:30 Paper 390a: ModCell: A Prototype for Modular Cell Engineering — *Donovan S. Layton, Brandon Wilbanks, Sergio Garcia,* ***Cong T. Trinh***

12:48 Paper 390b: A Synthetic Biosensor to Determine Peroxisomal Acetyl-CoA Concentration for Compartmentalized Metabolic Engineering — ***Herbert Huttanus***, *Jiayuan Sheng, Xueyang Feng*

1:06 Paper 390c: Tailoring Pathways for Balanced Expression by Short Mufflers — ***Carmen Lopez-Garcia***, *Zengyi Shao*

1:24 Paper 390d: Development of a Formaldehyde Biosensor and Its Application to Engineering of Methanol Metabolism in *E. coli* — ***Benjamin Woolston***, *Timothy Roth, David R. Liu, Greg Stephanopoulos*

1:42 Paper 390e: Synthesis of Isobutanol and n-Butanol Using Engineered Coenzyme A–Dependent Pathways in *Ralstonia eutropha* H16 — ***William Black***, *Linyue Zhang, James C. Liao, Han Li*

2:00 Paper 390f: Layered Regulation Strategies to Improve D-Glucaric Acid Production — ***Stephanie J. Doong***, *Apoorv Gupta, Kristala Prather*

2:18 Paper 390g: Strategies for Exploiting Non-Growth Metabolism in Biosynthesis — ***Keith E. J. Tyo***

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(391) The Industrial Fluid Properties Simulation Challenge
Tuesday, Oct 31, 12:30 PM
MCC, L100H

Jonathan D. Moore, Chair
Daniel W. Siderius, Co-Chair

Sponsored by:
Computational Molecular Science and Engineering Forum

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(392) Thermophysical Properties and Phase Behavior I
Tuesday, Oct 31, 12:30 PM
MCC, L100J

Clare McCabe, Chair
Erik E. Santiso, Co-Chair

Sponsored by:
Thermodynamics and Transport Properties

12:30 Paper 392a: Area 1A Keynote Lecture (Invited Talk) — ***Sharon C. Glotzer***

1:15 Paper 392b: Prediction of Solid-State Phase Diagrams Using Multistate Reweighting and Jacobian Mapping — ***Natalie Schieber***, *Eric Dybeck, Nathan Abraham, Michael R. Shirts*

1:36 Paper 392c: Evaluation of Defect Concentrations in Crystalline Systems via Molecular Simulation — *Apoorva Purohit,* ***Andrew J. Schultz***, *Jeffrey Errington, David A. Kofke*

1:57 Paper 392d: Nature of the Instability of the Body-Centered-Cubic (bcc) Structure in Classical Hard Sphere Solids — *Vadim B. Warshavsky,* ***David M. Ford***, *Peter A. Monson*

2:18 Paper 392e: Entropy-Driven Solid–Solid Transitions in Colloids — ***Chrisy Xiyu Du***, *Greg van Anders, Richmond S. Newman, Sharon C. Glotzer*

2:39 Paper 392f: Calculation of Glass Transition Using Sanchez-Lacombe EOS — ***Margarete Roericht***, *Kirstin Taufertshöfer, Sabine Enders*

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(393) The Use of CFD in Simulation of Mixing Processes
Tuesday, Oct 31, 12:30 PM
MCC, 102D

Minye Liu, Chair
Justin Walker, Co-Chair

Sponsored by:
North American Mixing Forum

12:30 Paper 393a: Large Eddy Simulation of a Pipeline Rotor-Stator Mixer — ***Benjamin A. Minnick***, *Richard V. Calabrese*

12:51 Paper 393b: Mean-Age Distribution in General Time-Dependent Flows of Multiphases — ***Minye Liu***

1:12 Paper 393c: Calibration of Mean Age for Blend Time in Batch Processes — ***David C. Russ***, *Thomas Eppinger, Ravindra Aglave*

1:33 Paper 393d: Modeling the Residence Time Distribution in a Continuous Plug-Flow Reactor — ***Christopher Tyler***, *John Thomas*

1:54 Paper 393e: Analyzing Direct Numerical Simulation Data for a Marginally Turbulent Stirred Vessel Driven by a Rushton Turbine — *Niall O'Byrnes,* ***Harry E. A. Van den Akker***

2:15 Paper 393f: A New Mixing Model for Turbulent Reacting Flows Using Hierarchical Parcel Swapping (HiPS) — ***David O. Lignell***, *Alan Kerstein, Justin Ward, Alessandro Perego*

2:36 Paper 393g: Application of Computational Fluid Dynamics to Assess Scale-Up Risk to Manufacture Polymeric Resins for the Paints and Coatings Industry — ***Bradon J. Dreyer***, *Johnathan T. Gorke, Jeremy Patt, Alyssa Krutzig, Benjamin Bangasser, Daniel Caron*

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(394) Topical Plenary: Advances in Fossil Energy R&D (Invited Talks)
Tuesday, Oct 31, 12:30 PM
MCC, 200C

Madhava Syamlal, Chair
Chunshan Song, Co-Chair

Sponsored by:
Advances in Fossil Energy R&D

12:30 Paper 394a: Fossil Energy Policy in the Trump Administration — ***Barry Worthington***

1:05 Paper 394b: Emerging Technologies in Fossil Energy and Chemical Conversion — ***George Richards***

1:40 Paper 394c: University Coalition for Fossil Energy Research: A New DOE-NETL National Alliance for Clean Energy Solution — ***Chunshan Song***

2:15 Paper 394d: Reliance Energy R&D — ***Thomas Mathew***

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(395) Electrokinetics for Sample Preparation
Tuesday, Oct 31, 1:15 PM
Hilton, Marquette IV/V/VI/VII

Lisa A. Flanagan, Chair
Mei He, Co-Chair

Sponsored by:
2017 Annual Meeting of the AES Electrophoresis Society

1:15 Paper 395a: Colloidal Nanomaterials-Encapsulated Microcapsules for Biomolecular Sensing — ***Weixia Zhang***, *Xi Xie, Alireza Abbaspourrad, Daniel G. Anderson, David A. Weitz*

1:30 Paper 395b: Using Particle-Particle Interactions to Enable Challenging DEP Separations — ***Mario Saucedo-Espinosa***, *Blanca H. Lapizco-Encinas*

1:45 Paper 395c: Characterization of Streaming Dielectrophoresis Towards Rapid Particle Separation — ***Monsur Islam***, *Rucha Natu, Rodrigo Martinez-Duarte*

2:00 Paper 395d: Effect of Insulator Post Shape on Joule Heating Effects in Insulator-Based Dielectrophoretic Devices — ***Roberto C. Gallo-Villanueva***, *Victor H. Perez-Gonzalez, Blanca H. Lapizco-Encinas*

2:15 Paper 395e: Shear-Enhanced Microfluidic Platform for Antibody Purification, In-Situ Efficacy Testing, and Bio-Diagnostics
— ***Mehnaz Mursalat***, *Ayaa Belal, Natalija Tasovac, John Frederick, Tushar Gupta, Debjit Ghoshal, Nikhil Koratkar, K. Stephen Suh, Sagnik Basuray*

2:30 Paper 395f: AC Droplet Digital PCR — ***Zehao Pan***, *Yongfan Men, Satyajyoti Senapati, Hsueh -Chia Chang*

2:45 Paper 395g: Translating Prototype Research from Lab to Commercial Product — ***David Charlot***

3:00 Paper 395h: Point-of-Care Detection of Hematocrit in a Microfluidic System Integrating Microfabricated Carbon Electrodes
— *Hwi Yong Lee, Jessika A. Rogers, Chito Kendrick,* ***Adrienne R. Minerick***

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(396) Poster Session: Chemical Engineering Education
Tuesday, Oct 31, 3:15 PM
MCC, Exhibit Hall B

Benjamin J. Davis, Co-Chair
Matthew Liberatore, Co-Chair

Sponsored by: Education

Paper 396a: Developing Spreadsheet Skills Using an Interactive Material and Energy Balances Textbook
— ***Matthew Liberatore***

Paper 396b: Using Student-Developed Comics to Promote Learning of Transport Phenomena Concepts
— ***Jennifer Pascal***, *Tiffany Pascal*

Paper 396c: Nature-Inspired Chemical Engineering: Development of a New Course on an Emerging Topic
— ***Marc-Olivier Coppens***, *Daniel Lepek, Michele Lynch*

Paper 396d: The "Cilindro Rotador" as a Pedagogical Tool for Complex Engineering Systems — ***A. Nastasia Allred***, *J. Robby Sanders, Pedro E. Arce*

Paper 396e: Chem Quest: An Adaptive Pre-Freshman Online Chemistry Course
— ***Wean Sin Cheow***, *Prasad Iyer, Kok Hwa LIM*

Paper 396f: Peer Mentoring in Graduate School: Fostering Diversity to Achieve Scholarly Excellence
— ***Claudio Vilas Boas Favero***, *Shannon E. Moran, Omolola Eniola Adefeso*

Paper 396g: Developing a Graduate Student Professional Development Course — ***Tracy Carter***, *Hicham Fenniri*

Paper 396h: Increasing Student Knowledge Acquisition and Transfer Through the Use of Heuristics in a Team/Lab-Based Protein Engineering Course — ***Morgan Bocci***, *J. Robby Sanders, Pedro E. Arce*

Paper 396i: Re-Situating Learning and Shifting Culture in ChE at OSU
— Milo D. Koretsky, *Susan Nolen, Jim Sweeney, Michelle Bothwell, Devlin Montfort, Susannah Davis*

Paper 396j: A Cross-Discipline Heat Exchanger Project — ***Derek L. Englert***, *John F. Maddox*

Paper 396k: Faculty Incentives to Promote Active Learning
— ***Elizabeth Hill***, *Tracy Bibelnieks, Brian Gute, Alison Hoxie, David Saftner, Peter Willemsen, Kris Gorman, J.D. Walker*

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(397) Poster Session: Fundamentals and Applications of Adsorption and Ion Exchange
Tuesday, Oct 31, 3:15 PM
MCC, Exhibit Hall B

Daniel W. Siderius, Chair
Sasidhar Gumma, Co-Chair

Sponsored by:
Adsorption and Ion Exchange

■ GAS SEPARATIONS & COLUMN EXPERIMENTS

Paper 397a: Adsorption of PAHs on Al-MCM-41: Batch Equilibrium and Column Breakthrough Behavior
— *F. Murilo T. Luna,* ***Célio L. Cavalcante Jr***

Paper 397b: Effect of Different Epoxy Modifiers Applied to Amine–Silica Adsorbents for CO_2 Capture
— ***Jinseo Min***, *Sunbin Jeon, Sung Hyun Kim, Ki Bong Lee*

Paper 397c: Simulation Study of Capturing CO_2 from Syngas After Water-Gas Shift Reaction by Pressure Swing Adsorption
— ***Cheng-tung Chou***, *Wei-nung Huang, Chien-shun Chang, Hong-sung Yang*

Paper 397d: Effect of an Equalization Step on the Minimum Bed Size Factor of a Rapid Pressure Swing Adsorption Process — ***Aaron Moran***, *Orhan Talu*

Paper 397e: Reactive Fibrous Materials for the Sorption and Self-Decontamination of Chemical Threats
— *Lev Bromberg, Xiao Su,* ***Vladimir Martis***, *Yunfei Zhang, T. Alan Hatton*

Paper 397f: Low-Pressure Performance Evaluation of CO_2, H_2O and CH_4 on Li-LSX as a Superior Sorbent for Air Prepurification
— ***Franklin Epiepang***

Paper 397g: DMOF-1 as a Representative MOF for SO_2 Adsorption in Both Humid and Dry Conditions
— ***Julian T. Hungerford***

Paper 397h: Preparation and Its Selective Adsorption Property of Asphalt-Based Carbon Materials for Effective Separation of Light Hydrocarbons Methane/Ethane/Propane — ***Wanwen Liang***, *Huiyu Xiao, Daofei Lv, Jing Xiao, Qibin Xia, Zhong Li*

Paper 397i: Understanding the Performance of Slipped Covalent Organic Frameworks for CH_4 Storage and CO_2:CH_4 Separation Using Fixed-Bed Adsorption Column
— ***Abhishek Sharma***, *Ateeque Malani, Ravichandar Babarao, Nikhil Medhekar*

■ ION REMOVAL

Paper 397j: Study on the Adsorption Behavior of Activated Red Mud for Cr(VI) Ions from Aqueous Solution — *Lei Wang, Pengjie Gao, Shuqin Liang, Dan Zhang,* ***Jiang Su-yu***, *Li Hui-ping*

Paper 397k: Ultrasound-Assisted Synthesis of Zirconium-Impregnated Activated Carbon Nanocomposite and Its Effective Use for Defluorination of Water — ***Aditi Mullick***, *Sudarsan Neogi*

Paper 397l: Lithium-Selective 14-Crown-4 Ethers: Synthesis, Polymerization and Its Application for the Recovery of Lithium from Dilute Solutions — ***Rey Eliseo C. Torrejos***, *Grace M. Nisola, Jeong Woo Han, Seong-Poong Lee, Jeong Gil Seo, Wook-Jin Chung*

Paper 397m: Defluoridation of Water Using Amine-Functionalized Cellulose Nanofibers — ***Ramya Araga***, *Chandra S. Sharma*

Paper 397n: Uranium Adsorption on Organophosphorus-Derivatized Extractive Scintillating Resins
— ***Christine E. Duval***, *James C. Foster, Timothy A. DeVol, Scott M. Husson*

Paper 397o: Evaluation of Sugar Beet Processing Lime Cake for the Removal of Synthetic Dyes from Aqueous Solutions — ***Mustafa E. Marti***, *Hani Zeidan*

■ THEORY/MODELLING

Paper 397p: The Accuracy of Pore Size Distribution Obtained from Non-Local Density Functional Theory in Amorphous Microporous Materials: Polymers and Large Organic Molecules
— ***Grit Kupgan***, *Thilanga Liyana-Arachchi, Coray M. Colina*

Paper 397q: Gas Sorption and Swelling in Flexible Metal-Organic Frameworks
— ***Sahar Bakhshian***, *Muhammad Sahimi*

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(398) Poster Session: General Topics on Chemical Engineering I
Tuesday, Oct 31, 3:15 PM
MCC, Exhibit Hall B

Sipho C. Ndlela, Chair
David Reeder, Co-Chair

Sponsored by: Miscellaneous

■ CARBON DIOXIDE CAPTURE AND MANAGEMENT

Paper 398a: Investigation of CO_2 Desorption Performance in Tri-Solvent Blends (MEA-AMP-PZ) with and Without Catalyst — ***Xiaowen Zhang***, *Helei Liu, Zhiwu Liang*

Paper 398b: Fracturing Fluid Retention and its Effect on Fluid Flow in Microfractures of Tight Oil Reservoirs
— ***Zhaojie Song***, *Liya Zhang, Qingjie Liu, Zhiyao Chen, Jirui Hou*

Paper 398c: Validation of CFD Model for the Pilot-Scale Mineral Carbonation Bubble Column Reactor
— ***Minjun Kim***, *Seoung-Eon Park, Jonggeol Na, Chonghun Han*

Paper 398e: Sandstone Deformation by CO_2 Adsorption — ***Sahar Bakhshian***, *Muhammad Sahimi*

Paper 398f: CCUS Development in Middle China — ***Shuangxing Liu***

Paper 398g: Study of Kinetics, Solubility, Heat of Absorption and Formation of Bicarbonate and Carbamate of Linear and Ring Diamines in CO_2 Absorption Process
— ***Rui Zhang***, *Zhiwu Liang, Qi Yang, Xiao Luo*

Paper 398i: Thermokinetic Properties and Mass Transfer of CO_2 Absorption in Aqueous Benzylamine Solvents for CO_2 Capture — ***Satyajit Mukherjee***, *Amar N. Samanta, Syamalendu S. Bandyopadhyay*

Paper 398j: Process Modeling and Experimental Studies of a Novel Micro-Encapsulated Solvent System for CO_2 Capture — ***Goutham Kotamreddy***, *Ryan Hughes, Debangsu Bhattacharyya, Joshuah Stolaroff, Michael Matuszewski*

Paper 398k: CO_2 Capture Process Dynamic Design of Experiments and Model Validation
— ***Anderson Soares Chinen***, *Joshua C. Morgan, Benjamin P. Omell, Debangsu Bhattacharyya, David C. Miller*

Paper 398m: Construction and Intelligent Manipulation of Nanocarbon Composite Electrodes Toward Energy Storage and Mechanical Conversion Devices — ***Guan Wu Jr.***

Paper 398n: Design, Fabrication and Modification of Advanced Fluorescent Polymer Based on Ordered Quantum Dots from Nanoscale to Large Production — ***Su Chen***

Paper 398o: Differential Permeability Reduction of CO_2 and Water by Polymer Gel in Sandstone Rocks During Wag Process — ***Xindi Sun***, *Baojun Bai*

Paper 398r: Valuing Flexibility in CCS-Equipped Power Plants
— ***Clara F. Heuberger***, *Iain Staffell, Nilay Shah, Niall Mac Dowell*

Paper 398s: Computational Designing and Screening of Solid Materials for CO_2 Capture Technology
— ***Yuhua Duan***

Paper 398t: Mechanisms of Competitive Diffusion and Adsorption for CH_4 and CO_2 on Shale and Their Significance in Gas Transport in Shale Gas Reservoirs — ***Shupanxiang Chen***, *Zhiwu Liang*

Paper 398u: Development of Potassium- and Sodium-Promoted CaO Adsorbents for CO2 Capture at High Temperatures — ***Ahmed Al-mamoori***, *Fateme Rezaei*

■ HYDROGEN PRODUCTION AND STORAGE

Paper 398v: Inert-Substrate-Supported Tubular Single Cell for Direct Operation on Isooctane — ***Kai Zhao***, *Bok-Hee Kim, M. Grant Norton, Su Ha*

■ MEMBRANE-BASED SEPARATIONS

Paper 398w: Molecular Dynamics Simulations of Zeolite Nanosheets for Water Desalination — ***Li-Chiang Lin***, *Seyed Hossein Jamali, Thijs Vlugt*

Paper 398x: Prediction of Water Uptake in Ion-Exchange Membranes Using Gel Swelling Models
— ***Kentaro Kobayashi***, *Eui-Soung Jang, Ni Yan, Benny D. Freeman*

Paper 398z: Modelling Direct-Flow Hollow Fibre Membrane Filtration at Fixed Pump Driving Pressure
— ***Qian Xu***, *Robert W. Field*

Paper 398aa: A Highly Permeable Microporous Polyamide Membrane for Molecular Sieving of Nitrogen from Volatile Organic Compounds
— ***Haoli Zhou***, *Fei Tao, Quan Liu, Chunxin Zong, Wenchao Yang, Xingzhong Cao, Wanqin Jin, Nanping Xu*

Paper 398ab: Water Desalination Using Porous Organic Cage Membranes: A Simulation Exploration — ***Xian Kong***, *Jianwen Jiang*

Paper 398ac: A Molecular Simulation Protocol for Membrane Pervaporation
— ***Krishna Mohan Gupta***, *Jianwen Jiang*

Paper 398ad: Coordinate Immobilization of Silver Nanoparticles on Aminenated Polyethersulfone (AgNPs-APES) Composite Membrane for Prolonged and Constant Silver (Ag+) Release — ***Muhammad Salman Haider***, *Godlisten Shao, Hee-Taik Kim*

Paper 398ae: Use of Novel Reactor-Separator Combination (Membrane BioReactor) for Enzymatic Hydrolysis of Waste Fines and Fiber Rejects from Recycled Linerboard Paper Mills
— ***Surya Jampana***

Paper 398af: Boron-Nitride-Nanopore Membranes for Osmotic Power Harvesting — ***Sangil Kim***, *Aaditya Pdendse, Semih Cetindag, Sanjay Behura, Vikas Berry, Jerry Shan*

Paper 398ag: Molecular Insights on the Reverse-Selectivity Potential of Room-Temperature Ionic Liquid Membranes — ***Amir Khakpay***, *Farzin Rahmani, Sasan Nouranian, Paul Scovazzo*

Paper 398ah: Molecular Dynamics Simulation of Room-Temperature Ionic Liquid Membranes for CO_2/CH_4 and CO_2/N_2 Separations — ***Farzin Rahmani***, *Amir Khakpay, Sasan Nouranian, Paul Scovazzo*

Paper 398ai: Ionic Liquid–Based Methacrylate Polymer Membranes for Efficient Enrichment of 1,3-Propanediol from Fermentation Broths
— ***Harrison Hawkins***, *Lucas Boyd, C. Stewart Slater, Mariano Savelski, Iman Noshadi*

Paper 398aj: — ***Nitesh Bhuwania***, *Daniel Chinn*

Paper 398ak: Water Flow Inside Polyamide Reverse-Osmosis Membranes: A Nonequilibrium Molecular Dynamics Study
— ***Mingjie Wei***, *Yang Song, Yong Wang*

Paper 398al: On the Hydrodynamics and Mass Transport of Non-Newtonian Fluids in Spiral-Wound Membranes
— ***Mohamadali Masoudian***, *Natalie Germann*

Paper 398am: Intensification of the Enzymatic Hydrolysis of Recycled Paper Fiber Fragments Using Membrane Separations — ***Surya Jampana***, *Bandaru V. Ramarao*

■ SEPARATIONS

Paper 398an: Evaluation of the Efficiency in a Set of Air Separation Units Through Data Envelopment Analysis and Malmquist Productivity Index — ***David Fernández***, *Rubén Folgado, Laureano Jimenez Esteller,* ***Carlos Pozo Fernández***

Paper 398ao: Plantwide Control for Maximum-Throughput Operation of an Ester Purification Process
— ***Nitin Kaistha***

Paper 398ap: Crown Ether Diols Aerosol Cross-Linked with Poly(vinyl alcohol) as Specialized Li+ Adsorbent Nanofibers — ***Grace M. Nisola***, *Lawrence A. Limjuco, Rey Eliseo C. Torrejos, Jeong Woo Han, Khino J. Parohinog, Sangho Koo, Wook-Jin Chung*

Paper 398aq: Revitalization of 18-Year-Old Deceased Urea Stripper Offering Multiple Challenges and Marvels of Engro and Toyo Team
— ***Muhammad Salman Siddiqui***

Paper 398ar: Efficient Absorption of SO2 in Flue Gas by Environmentally Benign Functional Deep Eutectic Solvents — *Kai Zhang, Shuhang Ren, Yucui Hou, Ying Sun,* ***Weize Wu***

Paper 398as: Improving Secondary Drying Rates for Slow-Drying Amorphous Spray-Dried Dispersions
— ***Amber L. Broadbent***, *John Baumann*

Paper 398au: Energy-Integrated Natural Gas Liquid Recovery Process by Vapor-Recompressed Internally Driven Reboiler — ***Bandaru Kiran***

Paper 398av: Engineering Studies of the Effect of pH, Temperature and Protein Tertiary Structure on β-Lactoglobulin A and B Separation in Anion-Exchange Chromatography
— ***James T. Hsu***, *Gorgi Pavlov*

■ NANOTECHNOLOGY

Paper 398aw: Nano-Cellulose-Based Thin-Film Nanocomposite RO Membranes with Tunable Flux via Control of Interfacial Transport
— ***Ethan D. Smith***, *Stephen M. Martin*

Paper 398ax: Synthesis of 3D Na-Embedded Carbon Nanomaterials and Their Applications in Solar Cells
— ***Wei Wei***, *Yun Hang Hu*

Paper 398ay: Electrical Energy Generation via Reversible Chemical Doping on Carbon Nanotube Fibers
— ***Albert Tianxiang Liu***, *Yuichiro Kunai, Pingwei Liu, Anton Cottrill, Michael Strano*

Paper 398az: Observation of the Marcus Inverted Region of Electron Transfer from Asymmetric Chemical Doping of Pristine (n,m) Single-Walled Carbon Nanotubes — ***Albert Tianxiang Liu***, *Yuichiro Kunai, Anton Cottrill, Michael Strano*

Paper 398ba: Synthesis of Lithium Carbonate Nanoparticles Using an Upscaled Microfluidic Reactor
— ***Sashankha Tallapudi***, *Holly Stretz, John Massingill Jr.*

Paper 398bb: Bijel-Derived Nanocomposite Membranes for Advanced Separations
— ***Martin F. Haase***, *Kathleen J. Stebe, Daeyeon Lee*

Paper 398bc: Preparation of Nanoporous Silica with AgNPs at the Core and Crust to Control the Ag+ Ion Release and Enhance the Antibacterial Properties — ***Muhammad Salman Haider***, *Godlisten Shao, Hee-Taik Kim*

Paper 398bd: Development of Yttrium Nanoparticle/PVA-Modified PSf Membrane and Application in Decontamination of Arsenate from Waters — *Yang Yu, Ling Yu,* ***J. Paul Chen***

Paper 398be: Combined Molecular Confinement and Metal-Support Interface Effects for Control of Hydrodeoxygenation Selectivity on Porous Pd@TiO_2 — ***Bingwen Wang***, *Jing Zhang, J. Will Medlin, Eranda Nikolla*

Paper 398bf: Examining Effects on Bending Elasticity and Structure of Phospholipid Bilayer Membrane in Presence of Embedded Surface-Functionalized Inorganic Nanoparticles
— ***Saptarshi Chakraborty***, *Michihiro Nagao, Christopher L. Kitchens*

Paper 398bg: In-Situ Isolation of Bacteria Using Microfluidic Devices
— ***Clara Romero Santiveri***, *Nil Tandogan, Edgar D. Goluch*

Paper 398bh: Tailoring Pore Topology to Polymorphism by Engineering Metal Oxide Interfaces During Templating of Nanostructure Materials
— *Daniel Gregory, Qianying Guo, Li Lu, Christopher J. Kiely,* ***Mark A. Snyder***

Paper 398bi: Protein Nanocage: A Versatile Molecular Carrier
— ***Sierin Lim***

Paper 398bj: Supported, Homogeneously Alloyed Bimetallic Nanoparticles by Electrostatic Adsorption — ***Andrew Wong***, *Qiuli Liu, John R. Regalbuto*

TECHNICAL SESSIONS 2017

Paper 398bk: One-Step Synthesis of Carbon Nanotube-Supported Fischer-Tropsch Catalysts via Liquid-Injection Chemical Vapor Deposition — ***Xu Li***, *Haider Almkhelfe, Keith Hohn, Placidus B. Amama*

Paper 398bl: Characterization of Aluminum Carbide in Aluminum-Graphene Nanocomposites — ***Aditya Nittala***

Paper 398bm: 3D Vertically Aligned CNT/Graphene Hybrids from Layer-by-Layer Transfer for Supercapacitors — ***Enoch Nagelli***, *Liming Dai*

Paper 398bn: Oligodendrocyte Precursor Cell Maturation in a 3D Hydrogel System Through the Incorporation of Drug Delivery Nanoparticles or Topographical Cues (Grad Student Award) — ***Lauren Russell***, *Meghan Pinezich, Kyle Lampe*

■ POLYMERS, PLASTICS, AND COMPOSITES

Paper 398bo: Functionalized Graphene/Polyimide Thermal Conductivity Composites via Electrospinning–Hot Press Technique — ***Yongqiang Guo***, *Zhaoyuan Lv, Qiuyu Zhang, Yalan Wu, Junwei Gu*

Paper 398bp: Multicolored Triboluminescent Composites for Wind Utilization and Lubrication Failure Warning — ***Zhaofeng Wang***, *Hua Xu, Fu Wang, Yumiao Li*

Paper 398bq: Secondary Cell Electrode Application of Carbonized Polyimide Aerogel with Elaborate Structure — ***Jinyoung Kim***, *Gunhwi Kim, Daero Lee, Haksoo Han*

Paper 398br: Mimicking Nature: Mechanical Properties of Ultrastretchable, Silica-Based Synthetic Spider Webs Fabricated via 3D Printing — ***Marius Rutkevicius***, *Mackenzie Geiger, Dishit Parekh, Taylor Neumann, Michael D. Dickey, Saad A. Khan*

Paper 398bs: Zwitterionic Conjugated Polymers and Their Application in Biosensing — ***Gang Cheng***

Paper 398bt: Novel Environmentally Benign Hydrogel: Nano-Silica Hybrid Hydrolyzed Polyacrylamide/ Polyethyleneimine Gel System for Conformance Improvement in High-Temperature, High-Salinity Reservoir — ***Yifu Long***

Paper 398bu: COMPOSELECTOR: A European H2020 Project for Integrating Multiscale Material Simulation and Industrial Business Decisions — ***Erik Laurini***, *Maurizio Fermeglia, Domenico Marson, Sabrina Pricl*

Paper 398bv: Single-Step Catalytic Conversion of Propane to Propylene via Reactive Separation — ***Dolly Chitta***, *Matthew Lemieux*

Paper 398bw: Crystallization and Foaming Behaviors of Modified Polypropylene by Phenyl-Contained Function Group — ***Cong Li***, *Lian-Fang Feng, Xue-Ping Gu, Cai-Liang Zhang*

(399) Poster Session: General Topics on Separations
Tuesday, Oct 31, 3:15 PM
MCC, Exhibit Hall B

Stephen Ritchie, Chair
Alice Z. He, Co-Chair

Sponsored by: General Topics and Other Methods

Paper 399a: Hydrogen Sulphide Absorption Performance in Various Amines Solution for Combined Desulphurization and Dehydration — ***Usman Shoukat***, *Diego D. D. Pinto, Hanna Knuutila*

Paper 399b: An Investigation on Chemical Absorbents for the Effective Removal of Hydrogen Sulfide from Crude Oils — ***Tracy J. Benson***, *Obakore Agbroko, Karishma Piler*

Paper 399c: Hydrophobic Deep Eutectic Solvents: Their Discovery and Design for Separations — ***Dannie J. G. P. van Osch***, *Lawien F. Zubeir, Dries Parmentier, Adriaan van den Bruinhorst, Carin H. J. T. Dietz, Marisa A. A. Rocha, Nicole M. W. van der Heijden, Mark Vis, A. Catarina C. Esteves, Jaap van Spronsen, Remco Tuinier, Maaike C. Kroon*

Paper 399d: Thickening of Liquid Digestate: Integration of Vacuum Evaporator into a Biogas Plant — ***Marek Vondra***

Paper 399e: Process Optimisation in the Retreatment of Gold-Bearing Sand Dumps: A Case Study of Zimbabwe — *Gwiranai Danha, Nkosikhona Hlabangana,* ***Nonhlanhla G. Mguni***, *Diane Hildebrandt*

Paper 399f: Research on Separation Performance of Supersonic Separator with a Forward Helical Guide Blade — ***Huirong Liang***, *Shuai Zhang, Kegang Ling, Sai Wang*

Paper 399g: The Influence of Microstructure on Membrane Distillation: Accurate 3-D Reconstructions for Analysis of Pore-Scale Phenomena — ***Spencer Gilleon***

Paper 399h: Fabrication of PVDF/ PVDF-HFP-Blend Hollow Fiber Membranes for Direct-Contact Membrane Distillation — ***Peng Wu***, *Lan Ying Jiang*

Paper 399i: Mitigation of Thin-Film Composite Membrane Biofouling via Immobilizing Nano-Sized Biocidal Reservoirs in the Membrane Active Layer — *Alireza Zirehpour, Ahmad Rahimpour,* ***Ahmad Arabi Shamsabadi***, *Masoud Soroush*

Paper 399j: Ethanolamine Separation by Nanofiltration: A Molecular Simulation Study — ***Krishna Mohan Gupta***, *Qi Shi, Jianwen Jiang*

Paper 399k: Separation of Hexavalent Chromium Cr(VI) from Wastewater Through Supported Liquid Membrane Using Environmentally Benign Solvent — *Supriyo Mandal,* ***Prabirkumar Saha***

Paper 399l: Water-Stable Metal-Organic Framework–Based Adsorbent and Membrane for Precious Metal (Silver) Separation from Wastewater — ***Chenghong Wang***

Paper 399m: Fabrication of Dense ZSM-5 and Fe-ZSM-5 Membranes for High-Throughput Desalination — *Hongfeng Dong,* ***Xiufeng Liu***, *Hongyu Guo, Baoquan Zhang**

Paper 399n: Quantifying Bacterial Adhesion to Polymeric Membranes by Single-Cell Force Spectroscopy — ***Sara BinAmed***, *Anissa Hasane, Zhaoxing Wang, Santiago Romero-Vargas Castrillón*

Paper 399o: Ceramic Membrane–Based Technology for the Clarification of Mosambi And Orange Juice — ***Mihir K. Purkait***

Paper 399p: Nanoporous Crystals–Channeled Two-Dimensional-Material Membranes with Highly Enhanced Water Purification Performance — ***Kecheng Guan***, *Gongping Liu, Wanqin Jin*

Paper 399q: Two-Dimensional MXene Membrane for Water Purification — *Li Ding, Yanying Wei,* ***Haihui Wang***

Paper 399r: Nano-Structuring of UF and RO Membranes with Hydrophilic Polymers: Scalability of Membrane Synthesis via Atmospheric Pressure Plasma-Induced Graft Polymerization — ***Jie Zhang***, *Soomin Kim, Anditya Rahardianto, Yoram Cohen*

Paper 399s: Silica Scaling of RO Membranes: Real-Time Detection and Scaling Kinetics — *John Thompson, Anditya Rahardianto, Muhammad Bilal,* ***Yoram Cohen***

Paper 399t: Effect of Membrane Surface Chemistry on Water Permeance and Antifouling Properties — ***Nima Shahkaramipour***, *Cheng Kee Lai, Chong Cheng, Haiqing Lin*

Paper 399u: The Influence of Regional Variation in Packing Density upon Productivity and Membrane Fouling — ***Qian Xu***, *Robert W. Field*

Paper 399v: Fluoride Removal from Antarctic Krill (Euphausia superba) by Donnan Dialysis — ***Guojia Yan***, *Ming Tan*

Paper 399w: Fabrication of Crosslinked PAI/Speek Blend Membranes for Pervaporation Dehydration — ***Lan Ying Jiang***, *Ge Li*

Paper 399x: ZIF-67 Containing Mixed Matrix Membranes for Exceptional C_3H_6/C_3H_8 Separations — ***Heseong An***, ***Jong Suk Lee***

Paper 399y: High Performance Ultrafiltration Membrane with Cysteine-Functionalized Graphene Oxides for Sustainable Water Production — ***Saerom Kong***, *Min-Young Lim, Huiseob Shin, Jusung Han, Jongchan Lee*

(400) Poster Session: Particle Technology Forum
Tuesday, Oct 31, 3:15 PM
MCC, Exhibit Hall B

Manuk Colakyan, Co-Chair
Ray Cocco, Co-Chair

Sponsored by: Particle Technology Forum

Paper 400a: Numerical Approximation of a Population Balance Equation Involving Aggregation, Growth and Nucleation — ***Mehakpreet Singh***, *Gurmeet Kaur, Thomas De Beer, Ingmar Nopens*

Paper 400b: Interaction Between NO and Char in the Presence of Oxygen — *Wenxia Yan,* ***Songgeng Li***, *Cuigang Fan*

Paper 400c: Evaluation of 2MWe Oxy-Circulating Fluidized Bed Boiler Performance — *You Ra Gwak,* ***See Hoon Lee***

Paper 400d: In-Situ Desulfurization Behavior Under Oxy-CFB Boiler Conditions — *Ye Bin Kim,* ***See Hoon Lee***

Paper 400e: A Combined Experimental-Computational Study of Cohesive Powders Under Consolidation by XRCT Image Analysis and DEM Simulation — ***Andrew Abi-Mansour***, *Sean McClure, Michael Gentzler, Wenjuan Zheng*

Paper 400f: The Fabrication of Capillary Electrophoresis Microfluidic Chips with Metal Oxide Nanoparticles to Control Optical Properties — ***Matthew L. Hancock***, *Eleanor Hawes, Candace Gillette, Eric A. Grulke*

Paper 400g: Extended Thin-Film Electrocatalyst Structures via Pt Atomic Layer Deposition — ***William McNeary IV***, *Katherine Hurst, Shaun M. Alia, Scott A. Mauger, K. C. Neyerlin, Chilan Ngo, J. W. Medlin, Alan W. Weimer, Svitlana Pylypenko, Karen J. Buechler, Bryan S. Pivovar*

Paper 400h: Effect of Cluster Size and Voidage on Gas-Solid Behavior via CFD-DEM Simulation — ***Jiahui Zhou***, *Liqing Qin, Yingya Wu, Xingying Lan, Jinsen Gao*

Paper 400i: CPFD Simulation of Solids Residence Time and Mixing Behaviors in a Downer Reactor — ***Liqing Qin***, *Jiahui Zhou, Yingya Wu, Xingying Lan, Jinsen Gao*

Paper 400j: Settling Rate of Agglomerates Consisting of Polydisperse Primary Particles by Brownian Dynamics — *Anastasia Spyrogianni, Katerina S. Karadima,* ***Eirini Goudeli***, *Vlasis G. Mavrantzas, Sotiris E. Pratsinis*

Paper 400k: Particle Convection in Vibrating Bed — ***Satoru Matsuda***, *Yoshizo Suzuki, Hiroshi Takeda, Hiroki Oka, Hiroyuki Nawa*

Paper 400l: Atomically Deposited Sintering Aids: Assessing the Effects of Al_2O_3 Particle ALD on the Sintering and Performance of SOFC Electrolytes — ***Christopher J. Bartel***, *Rebecca O'Toole, Maila Kodas, Sandrine Ricote, Neal P. Sullivan, Austin Drake, Alexa Horrell, Robert Hall, Charles B. Musgrave, Alan W. Weimer*

Paper 400m: Greener Ethylene Production via Chemical Looping — ***Vasudev Pralhad Haribal***, *Luke Neal, Seif Yusuf, Fanxing Li*

Paper 400n: Control of Particle Structure and Size Distribution by Humidity — ***Georgios A. Kelesidis***, *Florian M. Furrer, Eirini Goudeli, Max L. Eggersdorfer, Karsten Wegner, Sotiris E. Pratsinis*

Paper 400o: Transition Metal Oxide Powders Made from Flame Spray Pyrolysis for Li-Ion Batteries — *Jinyun Liao, Taylor Smith, Khaleel Hamad,* ***Yangchuan Xing***

Paper 400p: Drag Model Evaluation Through Fluidized Beds and Free-Falling Particles — ***Kevin E. Buettner***, *Dmitry Portnikov, Haim Kalman, Jennifer Sinclair Curtis*

Paper 400q: Numerical Evaluation of Solid-Liquid Drag Models for a Fluidized-Bed Bioreactor — ***Daniela M. Koerich***, *Gabriela C. Lopes, Leonardo M. Rosa*

Paper 400r: Influence of Alumina Support Crystallinity on ALD-Synthesized Cobalt Catalysts for Fischer-Tropsch Synthesis — ***Jacob M. Clary***, *Staci A. Van Norman, Dong Su, Eric A. Stach, John L. Falconer, Charles B. Musgrave, Alan W. Weimer*

Paper 400s: Experimentally Validated Discrete Element Model to Predict Pharmaceutical Powder Flow at Different Humidity Conditions — ***Raj Mukherjee***, *Sayantan Chattoraj, Chen Mao, Bodhisattwa Chaudhuri*

Paper 400t: Heat Transfer in a Rotary Drum Using Experiments and Simulations — ***Manogna Adepu***

Paper 400u: Single Drop Impact on Heterogeneous Powder Beds — ***Tianxiang Gao***, *Arun Sundar S. Singaravelu, Nikhilesh Chawla, Heather N. Emady*

Paper 400v: Drag Coefficients of Irregularly Shaped Particles — ***Fanhao Deng***, *Xiaoling Chen, Yongxing Zhang*

Paper 400w: Influence of Flow Hydrodynamics on Pyridine Synthesis Reaction — ***Shuaishuai Zhou***, *Mengxi Liu, Chunxi Lu*

Paper 400x: Fluidized Bed Rheology I: Fundamentals — ***Denis Schütz***, *Elke Riedl, Abhishek Shetty, Katja Hartmann*

Paper 400y: Investigation of the Agglomeration Behaviors in Gas-Solid Fluidized Beds with Side-Wall Liquid Injecting — ***Qiang Shi***, *Shaoshuo Li, Sihang Tian, Zhengliang Huang, Jingdai Wang, Yongrong Yang*

Paper 400z: Industrially Relevant Powder Characterisation Using a Uniaxial Powder Tester — ***Tim Freeman***, *John Yin, Katrina Brockbank*

Paper 400aa: Using Magnetically Assisted Impact Coating (MAIC) to Improve Powder Flow Parameters — ***Charles R. Bowman***, *Tim Freeman, William A. Hendrickson, Christopher J. Rueb, Robert G. Bowman, Katrina Brockbank, Jamie Clayton*

Paper 400ab: Influence of Acoustic Waves on the Solids Distribution in a CFB Riser — *Vivien Rossbach,* ***Jonathan Utzig***, *Agenor Furigo Jr., Henry F. Meier, Cíntia Soares*

Paper 400ac: Investigation of Humidity Effects on Electrostatic Behavior of a Small Cold Model Fluidized Bed — *Petteri Sippola,* ***Jari Kolehmainen***, *Ali Ozel, Xiaoyu Liu, Pentti Saarenrinne, Sankaran Sundaresan*

Paper 400ad: BubbleTree: A Rigorous Algorithm for Lagrangian Tracking and Statistical Analysis of Bubble or Cluster Motion within 3D Fluidized Bed Simulations — *Kyle Buchheit, Christos Altantzis,* ***Akhilesh Bakshi***, *Terry Jordan, Dirk Van Essendelft*

(401) Poster Session: Separations Division
Tuesday, Oct 31, 3:15 PM
MCC, Exhibit Hall B

Mark M. Davis, Chair
Scott M. Husson, Co-Chair

Sponsored by: Separations Division

■ DISTILLATION & ABSORPTION

Paper 401a: Unique Design Considerations for Maximum-Boiling Azeotrope via Extractive Distillation System: Acetic Acid/N,N-Dimethylacetamide Separation — ***Yen-Hsiang Wang***, *Ka-Man Lo, I-Lung Chien*

Paper 401b: Separation and Purification of Cyclopentadiene and Methyl Cyclopentadiene from Pyrolysis Carbon 9 — ***Yu-Fei Wang***

Paper 401c: Purification of Styrene from the Styrene/Xylene Mixture by a New Technique Combining Distillation and Crystallization — ***Lie-Ding Shiau***

Paper 401d: Performance Evaluation of Long-Chain Alkyl Ionic Liquids and Their Mixtures for CO_2 Solubility at Elevated Temperature and Pressure — ***Ruh Ullah***, *Tausif AlTamash, Majeda Khraisheh Sr.*

Paper 401e: Capture of Nitric Oxide in Simulated Flue Gas by a Metallic Functional Ionic Liquid — *Ying Sun, Shuhang Ren, Yucui Hou, Kai Zhang,* ***Weize Wu***

■ CRYSTALLIZATION & EVAPORATION

Paper 401f: Vaporization of a Single N-Pentane Liquid Drop in a Flowing Mmicsible Liquid Media — ***Hameed B. Mahood Al-Muhammedawi***, ***Ali Sh. Baqir***, ***Makki Maliki***

■ EXTRACTION

Paper 401g: Extraction of Phenolics from Coal by Deep Eutectic Solvents — ***Kyle McGaughy***, *Bishwadeep Bagchi, Nepu Saha, M. Toufiq Reza*

Paper 401h: Efficient Extraction Phenolic Compounds from Oil Mixtures with Inner Salts — *Congfei Yao, Yucui Hou, Shuhang Ren, Youan Ji,* ***Weize Wu***

Paper 401i: Efficient Decolorization of Citric Acid Fermentation Broth Using Carbon Materials Prepared from Phosphoric Acid Activation of Hydrothermally Treated Corncob — *Taotao Qin,* ***Jinglan Wu***, ***Hanjie Ying***

Paper 401j: Recovery of Monosaccharides from Dilute Acid Corncob Hydrolyzate Based on Nanofiltration Technology: Modeling and Optimization — *Kangkang Jiang, Jinglan Wu,* ***Hanjie Ying***

■ MEMBRANE-BASED SEPARATIONS

Paper 401k: Organic-Inorganic Composite Membranes: Fundamental Study and Engineering Application — ***Wanqin Jin***

Paper 401l: Modeling of Structural Defects in MFI Zeolite Membranes — ***Sungwon Hong***, *Jungkyu Choi*

Paper 401m: Role of Electrokinetics in Glomerular Capillary Filtration: Toward an Artificial Kidney — ***A. Nastasia Allred***, *Samantha Blanton, J. Robby Sanders, Pedro E. Arce*

Paper 401n: Filling of Clay Nanoparticles into Thin-Film Nanocomposite Membranes to Improve Their Efficiency Toward Brackish Water Desalination — ***Mohammed Kadhom***, *Baolin Deng*

Paper 401o: Advanced Membrane Separation to Improve Efficiency of Thermochemical Conversion of Biomass — ***Michael Z. Hu***

Paper 401p: Antifouling Membranes by Surface Modification Using Hydrophilic Polymers — ***Nima Shahkaramipour,*** *Chong Cheng, Haiqing Lin*

Paper 401q: Chlorine-Tolerant Block Polymer Nanofiltration Membranes — ***Yizhou Zhang***, *Ryan Mulvenna, Bryan W. Boudouris, William Phillip*

Paper 401s: Mixed-Matrix Membranes with Improved Interfacial Morphologies via Supramolecular Interactions — ***Qinnan Zhang***, *Ruilan Guo*

TECHNICAL SESSIONS 2017

Paper 401t: Commercial Polymeric Membranes for Nuclide Separation Applications — ***Hyung-Ju Kim***, *Keun-Young Lee, Bum Kyoung Seo*

Paper 401u: A Systematic Investigation of Ionic Liquids as Effective Draw Solutes for Forward Osmosis — *Hana G. Zeweldi,* ***Lawrence A. Limjuco***, *Hanseung Kim, Wook-Jin Chung, Grace M. Nisola*

Paper 401v: Development of Robust, Ion-Selective Anion-Exchange Membranes Through Incorporation of Ionic Liquid Materials for Water Purification via Electrodialysis — ***Saloumeh Kolahchyan***, *Alexander M. Lopez*

Paper 401w: Sorption-Enhanced Mixed-Matrix Materials Comprising Palladium Nanoparticles and Polybenzimidazole for H_2/CO_2 Separation — ***Lingxiang Zhu***, *Deqiang Yin, Shailesh Konda, Mark T. Swihart, Haiqing Lin*

Paper 401x: Perfluoropolymers and Hydrocarbon Polymer Analogs with Pendant Rings for Gas Separation Membranes — ***Milad Yavari***, *Minfeng Fang, Yoshi Okamoto, Haiqing Lin*

Paper 401y: A Computational Study of Water Sorption and Its Effect on CO_2 Separation Performance in Graphene Oxide–Based Membranes — ***Myungsuk Lee***, *Gyeong Hwang*

Paper 401z: Novel Mixed-Matrix Membrane Using Metal-Organic Framework and Graphene Oxide for CO_2 Separation — ***Pradip Das***, *Sasidhar Gumma, B. Mandal*

Paper 401aa: Pilot Deposition of Zeolite-Y Nanoparticles on Polyethersulfone Substrate for Composite Membrane Fabrication in CO_2 Separation — ***Dongzhu Wu***, *Yang Han, Lin Zhao, Witopo Salim, Varun Vakharia, W. S. Winston Ho*

Paper 401ab: Carrier Saturation Phenomenon in Facilitated Transport Membrane for CO_2 Separation from Low-Concentration Sources — ***Dongzhu Wu***, *Yang Han, W. S. Winston Ho*

Paper 401ac: Improved Polyethersulfone Substrates for Composite Membranes in CO_2 Separation — ***Dongzhu Wu***, *Yang Han, Witopo Salim, Kai Chen, W. S. Winston Ho*

Paper 401ad: Polymeric Membrane Systems for CO_2 Capture from Flue Gas: A Techno-Economic Analysis — ***Yang Han***, *W. S. Winston Ho*

Paper 401ae: Membranes for CO_2 Capture from Low-Concentration Sources: A Technical and Economic Feasibility Study — ***Yang Han***, *W. S. Winston Ho*

Paper 401af: Polyelectrolyte-Modified Graphene Oxide/Polypropylene Composite Membranes for Organic Solvent Nanofiltration — ***Dan Hua***, *Tai-Shung Chung*

Paper 401ag: The Effects of Chemical Structure on Gas Transport Properties in a Family of Polyethersulfones Polymers — ***Ali Naderi***, *Yong Wai Fen, Youchang Xiao, Neal Chung, Martin Weber, Christian Maletzko*

Paper 401ah: High-Resolution Scalable Propylene/Propane Separation for ZIF-8 Polycrystalline Membranes on Ceramic Tubular Supports — ***Jingze Sun***, *Hae-kwon Jeong*

Paper 401ai: Cross-Linked Polyimides for Membrane H_2/CO_2 Separation at Elevated Temperatures — ***Maryam Omidvar***, *Mark T. Swihart, Haiqing Lin*

Paper 401aj: Preparation and Characterization of Zeolite-Polymer Mixed-Matrix Membranes Filled with KFI- and RHO-Type Zeolites — ***Cigdem Atalay-Oral***, *Melkon Tatlier*

Paper 401ak: Gas Separation from Intrinsic Defects of Single-Layer Graphene — *Kumar Varoon Agrawal, Shiqi Huang*

Paper 401al: Relationship Between pKa of Amines in Microgel Particle Membranes and CO2 Permeance — ***Tomohiro Gyobu***, *Ryutaro Honda, Kazushi Imamura, Chie Yamashita, Ikuo Taniguchi, Yoshiko Miura, Yu Hoshino*

Paper 401am: Effect of Moisture on Mechanical Properties of an Amphiphilic Block Copolymer Membrane — ***Daniel T. Hallinan Jr.***, *Onyekachi Oparaji, Suresh Narayanam, Alec Sandy*

Paper 401an: A High–Free Volume Pentiptycene-Based Polyimide for CO_2 Removal — ***Ahmad Arabi Shamsabadi***, *Farzad Seidi, Mohammad Nozari, Masoud Soroush*

Paper 401ao: The Effects of SiO_2 and Zeolite 4A/SiO_2 on the Transport Behavior of CO_2 and CH_4 Through Polydimethylsiloxane Nanocomposite Membranes — ***Emmanuel Ogbole***, *Jianzhong Lou, Shamsuddin Ilias*

Paper 401aq: Composite Ionic Liquid and Dense Polymeric Membranes for CO_2/N_2 and CO_2/CH_4 Gas Separation at Elevated Pressures — ***Majeda Khraisheh Sr.***

Paper 401ar: Chabazite SAPO-34 Zeolite Membranes for Krypton/Xenon Separation: Enhanced Separation Performance and Process Modeling —

Paper 401as: Metal-Organic Framework/Graphene Oxide Composite Fillers in Mixed-Matrix Membranes for CO_2 Separation — *Stavroula Anastasiou, Jeewan Pokhrel, Nidhika Bhoria, K. Suresh Kumar Reddy,* ***Georgios N. Karanikolos***

Paper 401at: Characterization of Composite Pd/Ta Metallic Membranes for Hydrogen Separation — ***Chan Hyun Lee***, *Young Suk Jo, Jonghee Han*

Paper 401bh: Cross-linked Highly Sulfonated Poly(arylene ether sulfone) Prepared by Thiol-ene Reaction for Fuel Cell Application — ***Jusung Han***, *Kihyun Kim, Junghwan Kim, Eunki Kim, Saerom Kong, Jongchan Lee*

Paper 401bi: Graphene Oxide-doped Polyethersulfone Hollow Fiber Membranes for Bioartificial Kidney Application — ***Akshay Modi***, *Surendra Kumar Verma, Jayesh R. Bellare*

Paper 401bj: Multi-stage Electrodialysis for Coal Chemical Industry Wastewater Treatment — ***Yaoming Wang***, *Haiyang Yan, Liang Wu,* ***Tongwen Xu***

■ ADSORPTION & ION EXCHANGE

Paper 401au: Adsorption Rate Constant and Equilibrium Constant in Chiral Separation for Trans-Stilbene Oxide, Linalool and Ibuprofen by Supercritical Fluid Chromatography — ***Kosei Yonezawa***, *Junichi Sakabe, Toshitaka Funazukuri*

Paper 401av: Prediction of Water Uptake in Ion-Exchange Membranes Based on Gel Swelling Models Combined with Ion Sorption Model — ***Kentaro Kobayashi***, *Eui-Soung Jang, Ni Yan, Benny D. Freeman*

Paper 401aw: Design of Ionic Liquid Epoxy-Functionalized Ion-Exchange Resin Wafers for Low-Energy Electrodeionization — ***Angela Fasuyi,*** *Alexander Lopez*

Paper 401ax: Research on CO_2 Sorption Capacity of Two Silica-PEI Samples in the Bubbling Fluidized-Bed Reaction System — ***Young Cheol Park***, *Jae-Young Kim, Jong-Ho Moon, Sung-Ho Jo, Seung-Yong Lee, Chang-Keun Yi, Hyunuk Kim, Jung Yoon Seo, Hyojin Lee, Colin E. Snape*

Paper 401ay: Separation of CO_2/N_2 Mixture Using MIL-101(Cr)/PVA Pellets by PSA Process — ***Satyannarayana Edubilli***, *Sasidhar Gumma*

Paper 401az: Adsorption and Desorption Breakthrough Behaviors of Carbon Dioxide, Nitrogen, Water Mixture over PEI-Silica Solid Sorbent in a Temperature-Programmed Oven — ***Jong-Ho Moon***, *Jung Yoon Seo,* ***Je-Min Woo***, *Hyunuk Kim, Sung-Ho Jo, Chang-Keun Yi, Dong-Ho Lee, Jong-Seop Lee, Colin E. Snape, Young Cheol Park*

Paper 401ba: Tailoring Porous Polymers for Adsorption and Catalytic Applications — ***Mohsen Ghafari***, *John D. Atkinson*

Paper 401bb: Chemical Separations for Improved Catalytic Upgrading of Fast-Pyrolysis Bio-Oils — ***Mi Lu***, *Michael Z. Hu*

Paper 401bc: Determination of Adsorption Equilibrium Constants from Experimental Chromatograms for Liquid Adsorption — *Yosuke Watanabe, Kazuyuki Chihara, Yoshimi Seida, Noriyoshi Sonetaka, Kenneth Noll, Haruki Itoh,* ***Eiji Furuya***

Paper 401bd: Recovery of Lactic Acid from the Pretreated Fermentation Broth Based on a Novel Hyper-Cross-Linked Meso-Micropore Resin — ***Mingkai Song***, *Jinglan Wu, Hanjie Ying*

Paper 401be: Development of CuCl-Supported Nanoporous Adsorbent Exhibiting High Performances (Adsorption Capacity and Selectivity) of Carbon Monoxide Separation, and Strong Resistance to Oxidation Under Atmospheric Condition — ***Kanghee Cho***, *Taesung Jung, Jeong-su Kim, Jong-Nam Kim, Hee-Tae Beum, Sang-Sup Han*

Paper 401bf: Synthesis of Highly Performing Nanoporous Carbon Adsorbent for Separation of Siloxane and Ammonia Impurities from Land-Fill Gas — ***Kanghee Cho***, *Hyung Chul Yoon, Hee-Tae Beum, Jong-Nam Kim*

Paper 401bg: Synthesis of Various Water Adsorbents with Controllable Adsorption Properties for Application of Water Adsorption Chiller — *Kanghee Cho, Hee-Tae Beum, Dong-Woo Cho, Hyung Chul Yoon,* ***Jong-Nam Kim***

(402) Poster Session: Transport and Energy Processes
Tuesday, Oct 31, 3:15 PM
MCC, Exhibit Hall B

Jason Bara, Chair

Sponsored by:
Transport and Energy Processes

Paper 186o: Analytical Analysis of Flow Distribution Uniformity As a Design Criteria for a Novel Micro Packed-Bed Bionic Reactor — ***Weiliao Liu***

Paper 402a: Macroscopic and Microscopic Modeling of a Lithium-Ion Cell with Solid-State Intercalation Effect — ***Shi-Chern Yen***, *Chyun-Yaw Lin*

Paper 402b: Radiation-Induced Grafted FEP-G-Polystyrene Membranes: Chemical Degradation and Quantum Chemical Simulation — ***Xue Li***, *Yang Zhao, Weiwei Li, Shubo Wang, Xiaofeng Xie, Vijay Ramani*

Paper 402c: Analyses on the Effect of Natural Gas's Supercooling Temperature on the Liquefaction Performance of PRICO Process — ***Dongjie Lv***, *Qin Wang, Qi Song, Jing peng Zhang*

Paper 402d: Understanding the Effect of Zinc and Achieving Long Cycle Life in Cu-Intercalated Bi-Birnessite/Zinc Batteries — ***Gautam G. Yadav***, *Xia Wei, Jinchao Huang, Joshua Gallaway, Damon Turney, Michael Nyce, Sanjoy Banerjee*

Paper 402e: Integration of Experiment and Modeling for Evaluation of Microalgae Culturing in Split Airlift Photobioreactor — ***Laith Sabri***, *Abbas Sultan, Muthanna Al-Dahhan*

Paper 402f: Local Flow Dynamics in Split Airlift Reactor (Experiment and Validation of CFD Simulations) — ***Laith Sabri***, *Abbas Sultan, Hayder Al-Naseri, Muthanna Al-Dahhan*

Paper 402g: Thermodynamic Analysis of an Integrated Ca-Cu Chemical Loop for Abatement of Ventilation Air Methane — ***Yongxing Zhang***, *Xiaoling Chen, Behdad Moghtaderi*

Paper 402j: Measurements of the Size Distribution and Concentration of Engineered Nanoparticles in Aqueous Media: Methods and Applications — ***Brian Mader***, *Mark Ellefson, Charlie Chan, Christine Loza*

Paper 402k: CFD Simulation and Analysis of Gas-Liquid Segmented Flow with Mass Transfer in Microfluidic Devices: Case Study of CO_2 Gas Solubility and Diffusivity Measurement in Aqueous NaCl Solution — ***Pradeep Vyawahare***, *Samira Abedi, Mark W. Vaughn, Fazle Hussain, Chau-Chyun Chen*

(403) Poster Session: Upstream Engineering and Flow Assurance
Tuesday, Oct 31, 3:15 PM
MCC, Exhibit Hall B

Mohammad Tavakkoli, Chair
Francisco M. Vargas, Co-Chair
Sandeep Verma, Co-Chair
Michael P. Hoepfner, Co-Chair
Sandhya Sundar Ram, Co-Chair
Vikram Subramani, Co-Chair

Sponsored by:
Upstream Engineering and Flow Assurance Forum

Paper 403a: Sand Agglomeration in Oil & Gas Reservoirs Using Polymers — ***Rui Yan Lee***, *Paul F. Luckham, Omar K. Matar, M. Shahrul Amir Zamberi, Navin S. Karam Chand*

Paper 403b: Characterization of Hydrate Slurry Transportability: Comparison of High-Pressure Rheometer Measurements with Industrial-Scale Flowloop Data — ***Ahmad Abdul Majid***, *Carolyn A. Koh*

Paper 403c: Alkylammonium Formate-Based Protic Ionic Liquids for Methane Hydrate Inhibition: Offshore Flow Assurance — ***Tausif AlTamash***, *M. Fahed Qureshi, Mert Atilhan, Majeda Khraisheh Sr.*

Paper 403d: Solid Nanoparticles as Hydrate Inhibitors — ***Ashwin Kumar Yegya Raman***, *Clint P. Aichele*

Paper 403e: Production Forecast and Surveillance Using Data-Driven Methods — ***Xinli Jia***, *Feifei Zhang*

Paper 403f: Asphaltene Precipitation from a Brazilian Crude Oil by CO_2 Injection or by Pressure Reduction — *Mauro de Azevedo Ribeiro Saab, Verônica de Jesus Pereira, Silvio Alexandre Beisl Vieira de Melo,* ***Paulo de Tarso Vieira e Rosa***

Paper 403g: Effect of 1-Pentanol on Wettability of Oil/Brine/Rock Systems — ***Yingda Lu***, *Nariman Najafabadi, Abbas Firoozabadi*

Paper 403h: Flow Assurance Issues Associated with Ice Deposition Under Freezing Conditions — ***Hongfei Xu***, *Ben Bbosa, Eduardo Pereyra, Michael Volk*

Paper 403i: Electrical Treatment of Waxy Crude Oil to Improve Low-Temperature Flowability — ***Chenbo Ma***, *Jinjun Zhang, Chaohui Chen, Kai Feng, Zixin Li, Xinyi Wang, Yingda Lu*

Paper 403j: A Transient, Two-Fluid Model for Slug Flow Characterization — ***Pietro Poesio***

Paper 403k: Three-Phase Equilibrium Computations for Hydrocarbon-Water Mixtures — ***Michael Connolly***, *Huanquan Pan, Hamdi Tchelepi*

Paper 403m: Artificial Intelligence Applications to Forecast Oil Production from Hydraulically Fractured Reservoirs — ***Palash Panja***, *Raul Velasco, Manas Pathak, Milind Deo*

Paper 403n: Development of a New Model and Evaluation of Various Methods of Predicting Dew-Point Pressure for Gas Condensate Reservoirs — ***Mutlaq Alarouj***, *Osamah Alomair, Adel Elsharkawy*

(404) Broadening Participation in Chemical Engineering: Outreach Efforts That Work
Tuesday, Oct 31, 3:15 PM
MCC, 101I

Zenaida Otero-Gephardt, Chair
Dennis O'Brien, Co-Chair
Taryn Bayles, Co-Chair
Selma Mededovic Thagard, Co-Chair
Belinda Akpa, Co-Chair

Sponsored by: Education

3:15 Introductory Remarks

3:20 Paper 404a: Panelist: Dennis O'Brien — Programs, Best Practices, and Lessons Learned — ***Dennis O'Brien***

3:50 Paper 404b: Panelist: Taryn Bayles — Programs, Best Practices, and Lessons Learned — ***Taryn Bayles***

4:20 Paper 404c: Panelist: Tony Butterfield — Programs, Best Practices, and Lessons Learned — ***Anthony Butterfield***

4:50 Panel Discussion

5:25 Concluding Remarks

(405) 2017 Practice Award
Tuesday, Oct 31, 3:15 PM
MCC, L100A

Robert W. McCabe, Chair
John R. Regalbuto, Co-Chair
Lars C. Grabow, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

3:15 Introductory Remarks

3:25 Paper 405a: UOP Advanced MTO Technology – A New Route for the Production of Light Olefins — ***Paul T. Barger***

3:45 Paper 405b: On the Reaction Mechanism and the Nature of the Active Site for Standard Selective Catalytic Reduction of NO_x on Cu/SSZ-13 Zeolites — ***Fabio H. Ribeiro***, *W. Nicholas Delgass, Rajamani Gounder, Jeffrey T. Miller, William F. Schneider, Aleksey Yezerets, Atish A. Parekh, Christopher Paolucci, Ishant Khurana, Jonatan D. Albarracin Caballero, John R. Di Iorio, Arthur J. Shih*

4:05 Paper 405c: Mechanisms for C-C Bond Cleavage and formation during Acrolein Production on a Mixed Metal Oxide Catalyst — *Linh Bui,* ***Aditya Bhan***

4:25 Paper 405d: Conversion of Methane to Methanol and Ethanol in a Single Reactor — *Chukwuemeka Okolie, Yimeng Lyu, Yasmeen Belhseine, Libor Kovarik, Mark Engelhard, Eli Stavitski,* ***Carsten Sievers***

4:45 Paper 405e: Controlling Catalyst Binding Strength: Improved Reactivity Using Bimetallic Overlayer Structures — ***Joseph H. Holles***

5:05 Paper 405f: The Roles of Re and Cs as Promoters for $Ag/\alpha\text{-}Al_2O_3$ in High Selectivity Ethylene Epoxidation Catalysts — ***John R. Monnier***, *Weijian Diao, Chris Digiulio, Melanie Schaal, Shuguo Ma*

(406) Advances in Catalysis for Hydrogen Production
Tuesday, Oct 31, 3:15 PM
MCC, 200C

Dushyant Shekhawat, Chair
Daniel J. Haynes, Co-Chair

Sponsored by:
Advances in Fossil Energy R&D

3:15 Paper 406a: Short-Contact-Time Catalytic Partial Oxidation of Methane over Rhodium Catalysts Supported on 3D-Printed Ceramic Supports — ***Corey A. Leclerc***, *Rohan Gudgila*

3:30 Paper 406b: Characterization of Ni-Substituted Pyrochlore Catalysts for the Dry Reforming of CH4 — ***Daniel J. Haynes***, *Dushyant Shekhawat, David A. Berry, Yimeng Chen, Katherine Rice, Clayton W. Loehn, James J. Spivey*

3:45 Paper 406c: Dry Reforming of Methane over Zr,Y-Modified Ni/Mg/Al Hydrotalcite Catalysts for Hydrogen and Carbon Monoxide Production — *Katarzyna Świrk, Maria E. Gálvez, Monika Motak, Teresa Grzybek, Patrick Da Costa*

4:00 Paper 406d: A Multicore-Shell Catalyst Derived from Ni Phyllosilicate@SiO_2 for Low-Temperature Dry Reforming of Methane: Confinement Effect Against Carbon Formation — ***Zhofueng Bian***, *S. Kawi*

4:15 Paper 406e: Mixed (Dry & Partial Oxidation) Reforming of Methane with a New Catalyst Derived from a Negative-Value Mining Residue Spinellized with Nickel — ***Frank Dega***, *Mostafa Chamoumi, Nadi Braidy, Nicolas Abatzoglou*

4:30 Paper 406f: Design of Robust and Efficient Diesel Autothermal Reforming System Using Bi-Metallic Catalyst for the Mobile Applications — ***Jiwoo Oh***, *Jaemyung Lee, Joongmyeon Bae*

4:45 Paper 406g: Core-Shell Ni-Phyllosilicate@CeO_2 Catalyst with Excellent Coke Resistance in Steam Reforming of Biomass Tar — ***Sonali Das***, *Zhofueng Bian, Muhammad Hazim Rosli, Sibudjing Kawi*

5:00 Paper 406h: Synthesis of Three-Dimensionally Ordered Macroporous $La_{1-x}Ce_xNi_{03-\delta}$ as the Catalyst for Ethanol Steam Reforming — *Jingjing Shao,* ***Yongdan Li***

5:15 Paper 406i: Thermocatalytic Decomposition of Methane to Hydrogen and Carbon Nanotubes in Fluidized-Bed Reactor Using Ni-Based, Cu-Zn-Promoted and Alumina-Supported Catalyst — ***Kaushal Parmar***, *K. K. Pant, Shantanu Roy, Peddy V. C. Rao*

5:30 Paper 406j: The Modeling and Validation of CO Preferential Oxidation (CO PROX) Multi-Reactor System Using CuO/Rare Earth–Doped Ceria Catalysts for Commercial Diesel Reforming Applications — ***Jiwoo Oh***, *Joongmyeon Bae*

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(407) Advances in Chemical and Nuclear Process Safety
Tuesday, Oct 31, 3:15 PM
MCC, 200D

Thong Hang, Chair
John Olson, Co-Chair
Tinh Tran, Co-Chair

Sponsored by:
Nuclear Engineering Division

3:15 Paper 407a: Hazard Analysis Under Nuclear Regulations — ***Tinh Tran***

3:40 Paper 407b: Model-Predictive Safety System for Predictive Detection of Operation Hazards — *Masoud Soroush,* ***Jeffrey E. Arbogast***, *Warren D. Seider*

4:05 Paper 407c: Radiological Implications of the Physicochemical Form of Strontium Released During Postulated Nuclear Waste Facility Accident Conditions — ***Kevin R. O'Kula***, *David C. Thoman, Maeley K. Brown, Tinh Tran*

4:30 Paper 407d: Assessing Consequences of Chemical Releases on Control Room Habitability Using Habit 2.1 — ***Thomas O. Spicer III***, *Casper Sun, Syed I. Haider*

4:55 Paper 407e: Modeling of Self-Heating in Anion-Exchange Columns for Plutonium Recovery — ***James E. Laurinat***

5:20 Paper 407f: Effect of Cooling on Natural Circulation Velocity and Temperature Measurements Inside Vertical Heated Channel Representing Prismatic Modular Reactor Core — ***Mahmoud M. Taha***, *Ibrahim A. Said, Shoaib Usman, Muthanna Al-Dahhan*

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(408) Advances in Process Intensification
Tuesday, Oct 31, 3:15 PM
MCC, 101E

Robert Broekhuis, Chair
Chongwei Xiao, Co-Chair

Sponsored by:
Process Intensification & Microprocess Engineering

3:15 Welcoming Remarks

3:18 Paper 408a: Isolation of Low-Grade Biobased Bulk Chemicals — ***Daniela Painer***, *Susanne Lux, Matthäus Siebenhofer*

3:40 Paper 408b: An Efficient Approach for Chemical Process Development Using Kinetic Modeling in Batch and Continuous Mode — ***Marianna Katz***, *Nuno Torres, Filipe Ataíde, Carlos A. M. Afonso, Sílvia Pelicano, Nuno Matos*

4:02 Paper 408c: Intensification of Carboxylic Acid Isolation Processes by Emulsification — ***Andreas Toth***, *Robert Macher-Ambrosch, Susanne Lux, Matthaeus Siebenhofer*

4:24 Break

4:39 Paper 408d: Sustainable Pig Iron Production via Reduction of Mineral Iron Carbonate with Hydrogen — *Susanne Lux, Georg Baldauf-Sommerbauer,* ***Astrid Loder***, *Matthaeus Siebenhofer*

5:01 Paper 408e: A Novel Selective Ion Separation Process Using Battery System — ***Jeyong Yoon***, *Jaehan Lee, Seonghwan Kim, Seoni Kim, Hansun Yoon*

5:23 Paper 408f: Computational Investigation of Liquid Maldistribution in Periodically Operated Structured Packed Beds — ***Soumendu Dasgupta***, *Arnab Atta*

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(409) Anisotropic Particles: Synthesis, Characterization, Modeling, Assembly, and Applications
Tuesday, Oct 31, 3:15 PM
MCC, M100A

Ali Mohraz, Chair
Jaime Juárez, Co-Chair

Sponsored by: Interfacial Phenomena

3:15 Welcoming Remarks

3:18 Paper 409a: Engineering Shape Entropy for Colloidal Crystal Design — ***Yina Geng***, *Greg van Anders, Paul Dodd, Julia Dshemuchadse, Sharon C. Glotzer*

3:34 Paper 409b: Controlling Anisotropic Colloidal Assembly in External Fields — ***Isaac Torres-Diaz***, *Michael A. Bevan*

3:50 Paper 409c: Deposition Dynamics of Rod-Shaped Colloids During Transport in Porous Media — ***Huilian Ma, Ke Li***

4:06 Paper 409d: Engineering the Phase Behavior of Anisotropic Particles by Inverse Design — ***Chrisy Xiyu Du***, *Greg van Anders, Paul Dodd, Julia Dshemuchadse, Sharon C. Glotzer*

4:22 Paper 409e: Self-Assembly of Magnetic Janus Colloids via Brownian Dynamics Simulation — *Gabriel Vega-Bellido, Ronal A. DeLaCruz-Araujo, Ilona Kretzschmar,* ***Ubaldo M. Córdova-Figueroa***

4:38 Paper 409f: Brownian Dynamics of a Spherical Janus Particle near a Boundary as a Tool to Investigate TIRM — ***Aidin Rashidi***, *Christopher L. Wirth*

4:54 Paper 409g: Examining the Stability of Amphiphilic Janus Particle-Laden Interfaces — ***Ellen M. Knapp***, *Ilona Kretzschmar, Raymond Tu*

5:10 Paper 409h: Self-Assembly of Amphiphilic Janus Nanoparticles — ***Alan Hanley***, *Allan E. David*

5:26 Paper 409i: Magnetic Janus Particle Aggregation Rate at Long Times — ***Thomas Long***, *Ilona Kretzschmar, Joel Koplik*

5:42 Concluding Remarks

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(410) Area Plenary: Bionanotechnology II (Invited Talks)
Tuesday, Oct 31, 3:15 PM
MCC, 212A/B

Samantha A. Meenach, Chair
Kathryn A. Whitehead, Co-Chair
Millicent O. Sullivan, Co-Chair

Sponsored by: Bionanotechnology

3:15 Paper 410c: Improved Nonviral Gene Delivery Systems for Stem Cell Therapy and DNA Vaccination Applications — ***Angela K. Pannier***

4:05 Paper 410b: Nanoscale Interfacial Complexation in Emulsions (NICE): From Encapsulation and Release of Molecules and Cells to Recapitulating the Basic Functions of Living Cells — ***Daeyeon Lee***

4:55 Paper 410a: Development of Nanoparticulates Capable of Penetrating Physiological Barriers and the In-Vitro Systems Used for Their Analysis — ***Samantha A. Meenach***

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(411) Biomaterials: Graduate Student Award Session
Tuesday, Oct 31, 3:15 PM
MCC, 211D

Julianne L. Holloway, Chair
Adam Ekenseair, Co-Chair
Gulden Camci-Unal, Co-Chair
Bret Ulrey, Co-Chair

Sponsored by: Biomaterials

3:15 Paper 411a: A Two-Step Method for Transferring Single-Wall Carbon Nanotubes onto a Hydrogel Substrate — ***Mozhdeh Imaninezhad***, *Irma Kuljanishvili, Silviya Petrova Zustiak*

3:33 Paper 411b: Understanding How Lipid Nanoparticle Structure Affects Immune Response — ***Lisa Kasiewicz***, *Sushant Kumar, Rahul Purwar, Kathryn A. Whitehead*

3:51 Paper 411c: Photo-Induced Pinocytosis in Synthetic Liposomes — ***Danielle Konetski***, *Dawei Zhang, Christopher Bowman*

4:09 Paper 411d: Sugar-Coating the Answers to Virus Binding: Glycocalyx-Mimetic Interfaces — ***Ramya Kumar***, *Domenic Kratzer, Kenneth Cheng, Irina Kopyeva, Joerg Lahann*

4:27 Paper 411e: The Combined Effect of Matrix Microenvironment and Hypoxia on the Activity of Glioblastoma Stem Cells — ***Jee-Wei Emily Chen***, *Jann N. Sarkaria, Brendan A. Harley*

4:45 Paper 411f: Pegylated Poly(beta-amino ester) Delivery Systems for Periodic shRNA — ***Connie Wu***, *Wade Wang, Paula T. Hammond, Jiahe Li*

5:03 Paper 411g: Biodegradable Nano-Film-Coated Self-Floating Hollow Glass Microspheres for Rapid Cell Isolation and Recovery — ***Ziye Dong***, *Caroline Ahrens, Dan Yu, Zhenya Ding, Hyuntaek Lim, Wei Li*

5:21 Paper 411h: Enhancing Therapeutic Efficacy of Self-Assembling Prodrugs with Supramolecular Chemistry — ***Hao Su***, *Yuzhu Wang, Feihu Wang, Honggang Cui*

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(412) Carbon Dioxide Capture Technologies and Their Use
Tuesday, Oct 31, 3:15 PM
MCC, 102F

Sunil Hangal, Chair
Debangsu Bhattacharyya, Co-Chair

Sponsored by: Climate Change

3:15 Paper 412a: Electrochemical Swing Process for Carbon Capture — ***Sahag Voskian***, *T. Alan Hatton*

3:34 Paper 412b: Opportunities for Industrial CO2 Capture and Utilization in the US — ***Peter C. Psarras***, *Jennifer Wilcox*

3:53 Paper 412c: Improvement of Oxy-Combustion Using Thermodynamic and Exergetic Analysis — ***Renato P. Cabral***, *Niall Mac Dowell*

4:12 Paper 412d: Interfacial Speciation of CO_2-Loaded Aqueous Solutions of Alkanolamines — ***Naser S. Matin***, *Janice A. Steckel, Jesse G. Thompson, Moushumi Sarma, Kunlei Liu*

4:31 Paper 412e: Post-Combustion CO_2 Capture Using Hexamethylenediamine-Activated Aqueous Sodium Glycinate Solvent — *Bikash K. Mondal, Syamalendu S. Bandyopadhyay,* ***Amar Nath Samanta***

4:50 Paper 412f: Using Intellectual Property to Protect Carbon Capture Innovations — ***Charles Collins-Chase***, *Lauren Dowty*

5:09 Paper 412g: Whole-Systems CO_2 Value Chain Modelling: A Closer Look at the Pathways Through Syngas — ***Christopher Quarton***, *Sheila Samsatli*

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(413) Charged and Ion-Containing Polymers
Tuesday, Oct 31, 3:15 PM
MCC, 211B

Jessica Schiffman, Chair
Sarah L. Perry, Co-Chair

Sponsored by: Polymers

3:15 Paper 413a: Size-Selective Ionically Crosslinked Polymer Multilayer Films for Light Gas Separation — ***Jaime C. Grunlan***, *Benjamin Wilhite*

3:45 Paper 413b: Length Effects on Polyelectrolyte Complexation: How 'Poly' Must a Polyelectrolyte Be? — ***Jeffrey Vieregg***, *Michael Lueckheide, Matthew V. Tirrell*

4:00 Paper 413c: Interaction and Dynamics of Polyelectrolytes in Polyzwitterionic Complexes — ***Y. Elaine Zhu***, *Benxin Jing, Kehua Lin*

4:15 Paper 413d: Tuning Complex Coacervation Using Sequence-Defined Polyelectrolytes: A Molecular Understanding — *Tyler Lytle, Li-Wei Chang, Jason Madinya, Sarah L. Perry,* ***Charles E. Sing***

4:30 Paper 413e: Photodirected Assembly and Self-Rupture of Polyelectrolyte-Based Soft Materials — *Udaka K. de Silva, Amanda C. Bryant-Friedrich,* ***Yakov Lapitsky***

4:45 Paper 413f: Coarse-Grained Model for Polyelectrolyte Complexation — ***Marat Andreev***, *Samanvaya Srivastava, Lu Li, Matthew V. Tirrell, Jack F. Douglas, Juan de Pablo*

5:00 Paper 413g: Synthesis and Solution-Phase Characterization of Hydroxylated Sulfonated Oligothioetheramides — ***Joseph Brown***, *Christopher A. Alabi*

5:15 Paper 413h: Effect of Nanoparticle on the Structure and Dynamics of Model PEAA Ionomers from Molecular Dynamics Simulations — ***Janani Sampath***, *Lisa M. Hall*

5:30 Paper 413i: Zwitterionic Copolymers as Novel Supporting Scaffolds for Ionic Liquid-Based Gel Electrolytes — *Luis Rebollar, Fatin Lind,* ***Matthew J. Panzer***

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(414) Colloidal Hydrodynamics: Structure and Microrheology
Tuesday, Oct 31, 3:15 PM
Hilton, Marquette I/II/III/VIII/IX

Roseanna N. Zia, Chair
Travis W. Walker, Co-Chair

Sponsored by: Fluid Mechanics

3:15 Paper 414a: Using μ^2rheology to Characterize Consecutive Phase Transitions in a Hydrogenated Castor Oil Colloidal Gel — *Matthew Wehrman, Seth Lindberg,* ***Kelly M. Schultz***

3:45 Paper 414b: Hydrodynamic Entrainment in Micro-Confined Suspensions and Its Implications for Two-Point Microrheology — ***Christian Aponte-Rivera***, *Roseanna N. Zia*

4:00 Paper 414c: Shear-Induced Structural Ordering in Jammed Suspensions of Soft Particle Glasses — ***Fardin Khabaz***, *Tianfei Liu, Michel Cloitre, Roger T. Bonnecaze*

4:15 Paper 414d: Dynamic Simulation of Aging in a Hard-Sphere Colloidal Glass After Volume-Fraction Jumps — *Jialun Wang, Xiaoguang Peng, Xi Li, Gregory B. McKenna,* ***Roseanna N. Zia***

4:30 Paper 414e: A New Conformation Tensor-Based Macroscopic Model for Emulsions with Particle Inertia — *Paul M. Mwasame,* ***Antony N. Beris***, *Norman J. Wagner*

4:45 Paper 414f: Polyelectrolyte–Particle Flocculation in Complex Aqueous Solutions and Mixed Hydrodynamic Fields — ***Athena E. Metaxas***, *Nikolas A. Wilkinson, Cari S. Dutcher*

5:00 Paper 414g: From Filaments to Coils: Controlling the Dynamics of Linked Colloidal Particle Chains — ***Steve Kuei***, *Sibani Lisa Biswal*

5:15 Paper 414h: A Combined Experimental and Numerical Analysis of DNA-Functionalized Colloidal Particle Deposition in a Channel Flow — ***Young Ki Lee***, *Christopher Porter, John C. Crocker, Scott L. Diamond, Talid Sinno*

5:30 Paper 414i: Structural and Rheological Relaxation upon Flow Cessation in Colloidal Dispersions: Transient, Nonlinear Microrheology — ***Ritesh P. Mohanty***, *Roseanna N. Zia*

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(415) Computational Catalysis I: Fundamentals
Tuesday, Oct 31, 3:15 PM
MCC, L100E

Jean-Sabin McEwen, Chair
Michail Stamatakis, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

3:15 Paper 415a: The Surprising Accuracy of Dispersion-Corrected Ggas in the Prediction of Dissociation Barriers on Transition Metal Surfaces — ***Shaama Mallikarjun Sharada***, *Thomas Bligaard, Alan C. Luntz, Geert-Jan Kroes, Jens K. Nørskov*

3:33 Paper 415b: Adsorbate Vibrations on Transition Metal Surfaces: Applications and Theory — ***Joshua Lansford***, *Dionisios G. Vlachos*

3:51 Paper 415c: Genetic Algorithm Enhanced by Atomistic Neural Network: Pt Clusters at the H_2 Atmosphere as an Example — ***Geng Sun***, *Phillippe Sautet*

4:09 Paper 415d: Prediction of Chemisorption Energies by Gaussian Processes — ***Martin H. Hansen***, *Paul C. Jennings, Thomas Bligaard*

4:27 Paper 415e: New Computational Tools for High-Throughput Discovery in Transition Metal Catalysis — ***Terry Z. H. Gani***, *Jon Paul Janet,* ***Heather J. Kulik***

4:45 Paper 415f: More Accurate Depiction of Adsorption Energy on Transition Metals Using Work Function as One Additional Descriptor — ***Xiaochen Shen***, *Yanbo Pan, Bin Liu, Jinlong Yang, Jie Zeng, Zhenmeng Peng*

5:03 Paper 415g: Molecular Simulation Study of How the Structure of Liquid Water Affects the Free Energies of Adsorption and Reaction in Aqueous-Phase Heterogeneous Catalysis — ***Xiaohong Zhang***, *Rachel Getman*

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(416) Computational Methods in Biological and Biomedical Systems I
Tuesday, Oct 31, 3:15 PM
MCC, 103F

Stacey D. Finley, Chair
Nigel Reuel, Co-Chair
Ashlee N. Ford Versypt, Co-Chair

Sponsored by:
Applied Mathematics and Numerical Analysis

3:15 Paper 416a: Inter-Individual Variability in Physiological Response to Lipid Infusions Predicts Considerable Heterogeneity in Outcomes for Lipid Resuscitation: A Physiologically Based Pharmacokinetic-Pharmacodynamic Study in a Virtual Population — *Matthew McDaniel, Kevin Flores,* ***Belinda S. Akpa***

3:34 Paper 416b: Effect of Circadian Disruption on Hepatic Gluconeogenesis — ***Seul-A Bae***, *Ioannis P. Androulakis*

3:53 Paper 416c: A PK/PD Model of ACE Inhibition in Kidney Cells for Treatment of Diabetic Tissue Damage — ***Minu R. Pilvankar***, *Hui Ling Yong, Ashlee N. Ford Versypt*

4:12 Paper 416d: Dynamic Analysis of the DNA Sensing Pathway Predicts Host Immune Response — ***Robert W. Gregg***, *Saumenda N. Sarkar, Jason E. Shoemaker*

4:31 Paper 416e: Computational Modeling of Tuberculosis Granuloma Activation — ***Steve M. Ruggiero***, *Minu R. Pilvankar, Ashlee N. Ford Versypt*

4:50 Paper 416f: Investigating Cholera Toxin Binding Mechanism with Gangliosides via Kinetic Modeling and Experimental Measurements
*— **Dongheon Lee**, Singla Akshi, Hung-Jen Wu, Joseph Sangil Kwon*

5:09 Paper 416g: Biomarker Identification in Autism Spectrum Disorder: Common Pitfalls and Emerging Strategies
*— **Daniel P. Howsmon**, Troy Vargason, Uwe Kruger, Juergen Hahn*

5:28 Paper 416h: Stability Analysis of Stochastic Schlögl Model
*— **Michail Vlysidis**, Yiannis N. Kaznessis*

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(417) Conceptual Process Design in Refining, Petrochemicals and Gas Processing

Tuesday, Oct 31, 3:15 PM
MCC, 200A

Shu Wang, Chair
Saadet Ulas Acikgoz, Co-Chair
Tom Enright, Co-Chair

Sponsored by:
Fuels and Petrochemicals Division

3:15 Paper 417a: Energy Saving from Process Design: A Service-Oriented Architecture (SOA) Methodology
*— **Jia Li***

3:40 Paper 417b: Mathematical Modeling and Optimization of Commercial-Scale Catalytic Two-Stage, Ebullated-Bed, Direct Coal Liquefaction Reactors *— **Yuan Jiang**, Debangsu Bhattacharyya*

4:05 Paper 417c: Optimal Design of Pipeline System for Flare Minimization in Multiple Chemical Plants
*— **Yiling Xu**, Tianxing Cai, Wang Zhenlei, Qiang Xu*

4:30 Paper 417d: Development of a Natural Gas-to-Industrial Chemicals Bioprocess Platform *— **Bryan Yeh***

4:55 Paper 417e: Comparison of Conventional and Newly Proposed Solvent Deasphalting Processes: Numerical Simulation Based on Energy and Cost Analysis *— **Junwoo Park**, Soo Ik Im, Ki Bong Lee, Kang Seok Go, Nam Sun Nho*

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(418) Continuous Processing Technologies Applied in Drug Substance Development Chemistry

Tuesday, Oct 31, 3:15 PM
MCC, 204A/B

Mark Barrett, Chair
Joe Hannon, Co-Chair

Sponsored by:
Pharmaceutical Discovery, Development and Manufacturing Forum

3:15 Paper 418a: Overcoming Challenges for Scale-Up of Continuous Pharmaceutical Drug Substance Processes *— **Shujauddin M. Changi**, Donal Harrold, Harold Moloney, Martin D. Johnson, Scott A. May, Timothy M. Braden, Luke Webster, Joel Calvin, Carla Luciani*

3:37 Paper 418b: Preparation of Hazardous "On-Demand" Reagents Using Continuous Processing
*— **Sarah Rothstein**, Jerry S. Salan, David am Ende, Matthew Jorgensen, Trevor Rosensohn*

3:59 Paper 418c: Model-Aided Development for a Continuous Amide Bond Formation in a Drug Substance Manufacturing Process
*— **Derek Starkey**, Carla Luciani, Matthew C. Embry, Molly Hess, Justin Burt, David Mitchell*

4:21 Paper 418d: Effects of Catalyst and Metals Pretreatment for the Continuous Hydrogenation of a Halogenated Aromatic Nitro Compound
*— **Christopher Lippelt**, Jonas Y. Buser, Bradley M. Campbell, Richard F. Cope, Michael Laurila*

4:43 Paper 418e: Large-Scale Production of Pharmaceutical Intermediates in the Flow Mode
*— **Baoquan Sun**, Sam Tadayon*

5:05 Paper 418f: Plasmonic Metal Nanocatalysts as Platform for Continuous Synthesis of Drug Substances *— **Farshid Mohammadparast**, Andishaeh Dadgar, Marimuthu Andiappan*

5:27 Paper 418g: Developing Scale-Up Approach for Fast Reactions in Continuous Flow *— **Plamen Grigorov***

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(419) Design Under Uncertainty

Tuesday, Oct 31, 3:15 PM
MCC, 103C

Matthew D. Stuber, Chair
Ali Mesbah, Co-Chair
Zukui Li, Co-Chair
Brianna Christian, Co-Chair

Sponsored by:
Systems and Process Design

3:15 Paper 419a: A Surrogate-Based Method for Constrained Optimization with Black-Box Noisy Simulations
*— **Zilong Wang**, Marianthi Ierapetritou*

3:36 Paper 419b: Efficient Solution of Mixed-Integer Multistage Stochastic Programs for the Optimal Design of Smart Manufacturing Systems Using "Smooth-in-Expectation" Decision Rules *— Alphonse Hakizimana, **Joseph Scott***

3:57 Paper 419c: A Generalized Knapsack Problem–Based Decomposition Heuristic to Solve Large-Scale Multistage Stochastic Programs *— **Brianna Christian**, Zuo Zeng, Selen Cremaschi*

4:18 Paper 419d: Mixed-Integer Nonlinear Programming Models for Optimal Design of Reliable Chemical Plants *— **Yixin Ye**, Ignacio Grossmann, Jose M. Pinto, Sivaraman Ramaswamy*

4:39 Paper 419e: Network Design with Uncertain Edge Failures: Two-Stage Robust Optimization for Single-Commodity Networks
*— **Logan R. Matthews**, Chrysanthos E. Gounaris, Ioannis G. Kevrekidis*

5:00 Paper 419f: Robust Process Intensification and Optimization: Application to Carbon Capture Systems
*— **Michael Matuszewski**, Lorenz T. Biegler*

5:21 Paper 419g: Robust Optimization Using Polyhedral Norm and General Asymmetric Uncertainty Set
*— **Zukui Li***

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(420) Distributed Bioprocessing for Integrated Biorefineries

Tuesday, Oct 31, 3:15 PM
MCC, 101D

Nathan Mosier, Chair
John E. Aston, Co-Chair

Sponsored by:
Sustainable Biorefineries

3:15 Paper 420a: Economic and Energetic Analysis of Biofuel Supply Chains *— **Rex T. L. Ng**, Christos T. Maravelias*

3:40 Paper 420b: Synthesis of Sustainable Processing Networks: Location-Dependent Biorefinery Models
*— **Maria-Ona Bertran**, John M. Woodley, Rafiqul Gani*

4:05 Paper 420c: Electrochemistry as a Sustainable Alternative for Distributed Processing of Biomass *— **Luis A. Diaz**, Tedd Lister*

4:30 Paper 420d: Assessing Fuel and Feedstock Energy Use in the U.S. Chemical Sector: A Supply Chain Analysis *— **Scott Nicholson**, Alberta Carpenter, Rebecca Hanes*

4:55 Paper 420e: Beyond the Scientific Curiosity: Smart Use of Ionic Liquids in Integrated Biorefinery Concept
*— Andre M. da Costa Lopes, Roberto M. G. Lins, Ricardo A. Rebelo, **Rafal M. Lukasik***

5:20 Paper 420f: Integration of Fast Pyrolysis and Electrolyzer for Deoxygenation of Biomass
*— **Daniel Santosa***

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(421) Division Plenary: Food, Pharmaceutical, and Bioengineering Division (Invited Talks)

Tuesday, Oct 31, 3:15 PM
MCC, 208C/D

Michael C. Jewett, Chair
Rajanikanth Vadigepalli, Co-Chair

Sponsored by:
Food, Pharmaceutical & Bioengineering Division

3:15 Introductory Remarks

3:20 Food, Pharmaceutical and Bioengineering Division Distinguished Service Award in Chemical Engineering

3:25 Paper 421a: Food, Pharmaceutical and Bioengineering Division Award in Chemical Engineering: Directed Evolution of New Viruses for Therapeutic Gene Delivery
*— **David Schaffer***

4:05 Paper 421b: Area 15A Food Plenary Award - Efficient Biosynthesis of Microalgal DHA-Rich Oil: From Lab to Factory Scale *— **He Huang***

4:30 Paper 421c: Area 15B/PD2M Plenary Award: Biorelevant Phase Transformations in Supersaturated Solutions of Poorly Water Soluble Drugs
*— **Lynne S. Taylor***

4:55 Paper 421d: Area 15C Bioengineering Plenary Award: Orthogonal Metabolism for Industrial Biomanufacturing *— **Ramon Gonzalez***

5:20 Paper 421e: Area 15D/E Life Sciences Plenary Award: "Physiome on a Chip": How Integration of Systems Biology with "Organs-on-Chips" May Humanize Therapeutic Development
*— **Linda Griffith***

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(422) Electrocatalysis and Photoelectrocatalysis VI: Fuel Oxidation and Chemical Transformations

Tuesday, Oct 31, 3:15 PM
MCC, L100D

Eranda Nikolla, Chair
Marimuthu Andiappan, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

3:15 Paper 422a: Durable, Self-Hydrating, Tungsten Carbide-Based Composite Polymer Electrolyte Membrane Fuel Cells
*— **Weiqing Zheng,** Liang Wang, Stephen A. Giles, Yushan Yan, Ajay K. Prasad, Dionisios G. Vlachos*

3:33 Paper 422b: Improving Selectivity in Electrochemical Ammonia Synthesis
*— **Jay Schwalbe**, Aayush R. Singh, Joshua McEnaney, Adam Nielander, Thomas F. Jaramillo, Jens Nørskov, Matteo Cargnello*

3:51 Paper 422c: Teaching an Old Electrocatalyst to Do New Tricks
*— **Daniel V. Esposito**, Natalie Labrador, Eva Songcuan, Jacob Robinson, Bicheng Xu, Sophia Kurdziel*

4:09 Paper 422d: Using Surface Chemistry to Understand Aqueous-Phase Thermal Catalytic and Electrocatalytic Hydrogenation of Bio-Oil Model Substrates *— **Nirala Singh**, Udishnu Sanyal, John Fulton, Oliver Gutiérrez, Donald Camaioni, Charlie Campbell, Johannes A. Lercher*

4:27 Paper 422e: Design of Heterogeneous Catalysts for High-Temperature Electrochemical Reduction of CO_2
*— **Juliana S. A. Carneiro**, Xiang-Kui Gu, Zachary Kuczera, Eranda Nikolla*

4:45 Paper 422f: Enhancing Methanol Electrooxidation Activity Using Double Oxide Catalyst Support
*— **Ahmed Jasim**, Yangchuan Xing*

5:03 Paper 422g: Study of Impact of Electrode Catalyst Loadings on Thin Flexible Fuel Cell (TFFC) Performance
*— Seyed Reza Mahmoodi, Ronald S. Besser, **Matthew Mayer***

5:21 Paper 422h: Transition Metal–Modified Graphitic Mesoporous Carbon for PEMFC Application
*— **Khondker Sultana**, Dereje Worku, Md. Tashfin Zayed Hossain, Shamsuddin Ilias*

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(423) Fluidization and Fluid-Particle Systems for Energy and Environmental Applications I

Tuesday, Oct 31, 3:15 PM
MCC, 200I

Shyam Sundaram, Chair
Azita Ahmadzadeh, Co-Chair

Sponsored by:
Fluidization and Fluid-Particle Systems

3:15 Paper 423a: Multiscale Modeling of Biomass Thermochemical Conversion in Fluidized-Bed Reactors
*— **Himanshu Goyal**, Perrine Pepiot*

3:34 Paper 423b: Reduced-Order Particle-Scale Model for Biomass Pyrolysis and Gasification in Fluidized-Bed Reactors *— Giancarlo Gentile, **Akhilesh Bakshi**, Addison K. Stark, Christos Altantzis, Tiziano Faravelli, Ahmed F. Ghoniem*

3:53 Paper 423c: Numerical Investigation of Solid Residence Time Distribution in a Circulating Fluidized-Bed Riser for Catalytic Upgrading of Biomass Pyrolysis Vapors
*— **Xi Gao**, Tingwen Li, William Rogers*

4:12 Paper 423d: Thermal Desorption of Mercury from Coal Using a Draft-Tube Spouted Bed
*— **Nicholas R. Schwartz**, Michael J. Blaise, Paul E. Yelvington*

4:31 Paper 423e: Particle Circulation Motions in an Evaporating Droplet
*— **Lihui Wang**, Michael Harris*

4:50 Paper 423f: Fluidized Granular Activated Carbon (GAC) for the Mitigation of Membrane Fouling in Wastewater Treatment
*— Jingwei Wang, Anthony G. Fane, **Jia Wei Chew***

5:09 Paper 423g: Fluidized Bed Rheology II: Applications
*— **Abhishek Shetty**, Katja Hartmann, Denis Schütz*

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(424) Fundamentals and Applications for Municipal Solid Waste Treatment and Valorization

Tuesday, Oct 31, 3:15 PM
MCC, 102E

Eunsung Kan, Chair
Robert W. Peters, Co-Chair
Ramesh Chawla, Co-Chair

Sponsored by:
Solid and Hazardous Waste

3:15 Paper 424a: Effects of Household Co-Solvents on the Solubility and Oxidation of Trichloroethylene (TCE)
*— **Timara Benson**, Dhruba Paudel, Ramesh Chawla*

3:40 Paper 424b: Adsorptive Removal of Phosphorus from Wastewater Using Raw and Engineered Biochars
*— Yong-Keun Choi, Amado Maglinao, Sergio Capareda, **Eunsung Kan***

4:05 Paper 424c: Catalytic Gasification of Waste: A Sustainable Alternative
*— Eric M. Lange, **Uchechukwu Obiako**, Samuel Sanya, Stephen A. Reeves, Aliandra D. Barbutti, Jorge E. Gatica*

4:30 Paper 424d: Estimation of Energy Potential for Biogas Produced from Municipal Solid Waste (MSW) in Landfill of Astana Using Aspen Plus
*— **Mehdi Amouei Torkmahalleh**, Yerbol Sarbassov, Azat Myrzagaliev, Luis R. Rojas-Solórzano*

4:55 Paper 424e: Pyrolysis of Waste Plastics: A Modeling and Simulation Study on Pyrolysis Process for Synthesis Gas Production *— **Jithu K***

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(425) Fundamentals of Interfacial Phenomena II

Tuesday, Oct 31, 3:15 PM
MCC, M100B

Marina Tsianou, Chair
David Green, Co-Chair
Clint P. Aichele, Co-Chair
Bhuvnesh Bharti, Co-Chair
Younjin Min, Co-Chair

Sponsored by:
Interfacial Phenomena

3:15 Paper 425a: Capillary Foams: How a Small Amount of Oil Can Make a Big Difference *— **Yi Zhang**, Sven H. Behrens, J. Carson Meredith*

3:30 Paper 425b: Wetting on Strain-Induced Microstructured Surfaces
*— Vartika Parihar, Soumen Das, **Sunando DasGupta***

3:45 Paper 425c: Water Wetting on Surfaces Under Fuel Oil Containing Surfactants and Its Implication for Coalescence Separation of W/O Emulsions *— Qian Zhang, Yanxiang Li, Lixia Cao, Lei Li, **Chuanfang Yang***

4:00 Paper 425d: Stability of the Inertial Flow of Thin Liquid Film Inside a Uniformly Heated Rotating Horizontal Cylinder *— **Tara Chand Kumawat**, Naveen Tiwari*

4:15 Paper 425e: Dynamic Surface Tension Measurements of Ionic Surfactants Using Maximum Bubble Pressure Tensiometry
*— **Camilla U. Ortiz**, Vivek Sharma*

4:30 Paper 425f: First-Principles Analysis of Surface Terminations in Stoichiometric Metal Hexaborides
*— **Kevin Schmidt**, Olivia A. Graeve, Victor R. Vasquez*

4:45 Paper 425g: The Importance of Spreading Pressure on Adsorption-Based Surface Energy Measurements: The Case of IGC
*— **Eftychios Hadjittofis**, Geoff G. Z. Zhang, Jerry Heng*

5:00 Paper 425h: Stabilization of Glycerol/Dodecanol Pickering Emulsions with Surface-Grafted Silica Nanoparticles *— **Guolin Zhao**, Shuangliang Zhao Sr., Junyin Xiao, Honglai Liu, Marc Pera-Titus*

5:15 Paper 425i: In-Situ Observations of Dynamics of Active Braze Joining
*— **Anne M. Grillet**, Robert M. Garcia, David A. Barringer, Adam D. Martinez*

5:30 Paper 425j: High-Throughput Fabrication of Synthetic Asymmetric Bacterial Membranes
*— **Sepehr Maktabi**, Li Lu, Jeffrey W. Schertzer, Paul R. Chiarot*

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(426) Hydrogel Biomaterials

Tuesday, Oct 31, 3:15 PM
MCC, 209A/B

Mark W. Tibbitt, Chair
Kelly A. Burke, Co-Chair
Mozhdeh Imaninezhad, Co-Chair
Vamsi Yadavalli, Co-Chair

Sponsored by: Biomaterials

3:15 Paper 426a: Photoreversible Stiffness Modulation of Protein-Polymer Hydrogels *— Luman Liu, Jared A. Shadish, **Cole A. DeForest***

3:33 Paper 426b: Preparation and Characterization of Polypeptide Hydrogels as Synthetic Extracellular Matrices for Cellular Scaffolds
*— **Hongkun He**, Alex Wang, Marianna Sofman, Linda Griffith, Paula Hammond*

3:51 Paper 426c: Reinforced Hydrogel Fibers for Cell Encapsulation and Organ Printing *— **Suman Bose**, Daniel Anderson, Robert Langer*

4:09 Paper 426d: Synthesis and Applications of Environmentally Responsive Alginate Hydrogels
*— **Anuraag Boddupalli**, Kaitlin Bratlie*

4:27 Paper 426e: Novel Hydrogel Dressing Enhances Skin Wound Healing
*— **Lei Zhang***

4:45 Paper 426f: Magnetically Templated Hydrogels for Peripheral Nerve Injury Repair *— **Ishita Singh**, Christopher Lacko, Christine Schmidt, Carlos Rinaldi*

5:03 Paper 426g: A Two-Step Method for Transferring Single-Wall Carbon Nanotubes onto a Hydrogel Substrate *— **Mozhdeh Imaninezhad**, Irma Kuljanishvili, Silviya Petrova Zustiak*

5:21 Paper 426h: The Unique Mechanism of Covalently Adaptable Hydrogel Degradation Characterized with Passive Microrheology
— Francisco Escobar, Kristi S. Anseth, ***Kelly M. Schultz***

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(427) CO_2 Industrial, Engineering and R&D Approaches
Tuesday, Oct 31, 3:15 PM
MCC, 102C
Quinta Warren, Chair
Sipho C. Ndlela, Co-Chair

Sponsored by: Sustainability

3:15 Paper 427a: Increases in Demand for Fixed Nitrogen from Alternative Energy and Carbon Capture Schemes
— ***Luis F. Razon***

3:36 Paper 585ax: Pulse/Pulse-Reverse Electrodeposition of Copper Electrocatalysts for CO_2 Reduction to Ethylene — **Brian T Skinn**, *Sujat Sen, Rajeswaran Radhakrishnan, Steven M Brown, Stephen T Snyder, Fikile Brushett, Holly M Garich*

3:57 Paper 585v: Pilot Valve CFD Modelling — ***Bipin Kashid****, Aaron Morgan, Parsa Zamankhan, Xiao Hu*

4:18 Paper 398h: Multi-Objective Optimization of Solid Sorbent-Based CO_2 Capture Systems
— ***Miguel Zamarripa****, John Eslick, David C. Miller*

4:39 Paper 398p: Bioelectrosynthesis of Methane from CO_2 for Energy Storage *— Joshuah Stolaroff,* ***Sarah E. Baker****,* ***Jennifer M. Knipe****, Swetha Chandrasekaran, Marcus Worsley*

5:00 Paper 398d: Modeling the Sequestration and Transportation of CO_2 in Deformed Coalbed during Enhanced Coalbed Methane Recovery
— ***Quanshu Zeng****,* ***Zhiming Wang****,* ***Brian McPherson****, John McLennan*

5:21 Paper 398q: Integrated CO_2 Capture /Water-Gas Shift with Integrated HEAT Management for IGCC Applications *—* ***Shen Zhao****,* ***Andrew Lucero****, Santosh Gangwal*

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(428) Industrial Applications of Computational Chemistry and Molecular Simulation
Tuesday, Oct 31, 3:15 PM
MCC, L100H
Joseph T. Golab, Chair
Phillip R. Westmoreland, Co-Chair
Martin Sanborn, Co-Chair
Jonathan D. Moore, Co-Chair

Sponsored by:
Computational Molecular Science and Engineering Forum

3:15 Paper 428a: Top Ten Mistakes Applying Computational Chemistry in Industry *—* ***Brian K. Peterson***

3:45 Paper 428b: Atomic-Level Insights into Chemical Additives Used for Silicon-Containing Film Removal During Integrated Circuit Manufacturing
— ***Andrew J. Adamczyk****, Wen Dar Liu, Yi Chia Lee*

4:00 Paper 428c: Thiohypoiodous Acid (HSI) Formation and Its Role as an Intermediate in H_2 Production
— ***Phalgun Lolur****, Ryan J. Gillis, William H. Green*

4:15 Paper 428d: Computational Design of Thermodynamically Stable Metal Nanoparticles
— ***Giannis Mpourmpakis***

4:30 Paper 428e: Understanding the Geometrical and Electronic Properties of Imidazolium-Based Ionic Liquids in the Presence of Amino Acid Substituted Metal Porphyrins *—* ***Atiya Banerjee****, Jindal K. Shah*

4:45 Paper 428f: Towards the Prediction of the Liquid-Phase Oxidation of Aromatics: An Experimental and Modeling Study for Toluene Autoxidation
— ***Mickaël Matrat****, Detlev C. Mielczarek, Arij Ben Amara, Perrine Wund, Yvan Bouyou, Laurie Starck*

5:00 Paper 428g: Multiscale Molecular Dynamics Simulations of Asphaltenes in Crude Oils Based on the SAFT-γ Mie Force Field *—* ***Jason Law****, María Guadalupe Jiménez-Serratos, Erich A. Müller*

5:15 Paper 428h: Evaluating the Consistency and Accuracy of COSMO-RS-Based Free-Energy Predictions
— ***Jens Reinisch****, Andreas Klamt*

5:30 Paper 428i: Atomistic Simulation Studies of the Substitution Effect in Amine-Cured Epoxy Thermosets
— ***David Rigby***

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(429) Industrial Innovations Through Modeling and Optimization
Tuesday, Oct 31, 3:15 PM
MCC, 102B
Tom Xu, Chair
Shaibal Roy, Co-Chair
Raymond Wissinger, Co-Chair

Sponsored by:
Process Research and Innovation

3:15 Paper 429a: Modeling and Reaction Kinetics of Reactors for Polyesters Production
— ***Micaela Caramellino****, Eric Grolman*

3:40 Paper 429b: Modeling and Simulation of Nonwovens Manufacturing
— ***Alejandro Londono Hurtado***

4:05 Paper 429c: Some Studies on the Inherent Resilience for a Gas Sweetening Unit *—* ***Sirshendu Guha***

4:30 Paper 429d: Tubular Multi-Tube Cooled Reactor as a Fractional Heat Exchanger: Modeling Reactive Heat Transfer *—* ***Yihui Tom Xu***

4:55 Paper 429e: Thermal Stability of Ethylene Polymerization in Fluidized-Bed Reactor *—* ***Xiaoqiang Fan****, Zhengliang Huang, Jingdai Wang, Yongrong Yang*

5:20 Paper 429f: From Tool to Discipline: Developing a Model-Centric Process Engineering Culture
— ***Simon Padmanabhan****, Mehmet Morali, Debashis Chakraborty, Javier Nieves-Remacha, Gregory Hemmer*

5:21 Remarks from Former Students of Christos Georgakis

5:39 Concluding Remarks from Christos Georgakis

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(430) In Honor of Christos Georgakis's 70th Birthday
Tuesday, Oct 31, 3:15 PM
MCC, 103D
Fernando V. Lima, Chair
R. Donald Bartusiak, Co-Chair

Sponsored by:
Systems and Process Control

3:15 Paper 430a: Christos Georgakis: His Work and Legacy over 40 Years in Research and Education
— ***George Stephanopoulos***

3:33 Paper 430b: Optimal Control Laws for Batch and Semi-Batch Reactors Using the Concept of Extents
— Diogo Rodrigues, Julien Billeter, ***Dominique Bonvin***

3:51 Paper 430c: Extensive, Intensive and Invariant Variable Control Systems
— ***B. Erik Ydstie***

4:09 Paper 430d: Customer Feedback Control: Design and Implementation on a Nanocomposite Manufacturing Process *— Qian Gou, Mark D. Wetzel,* ***Babatunde A. Ogunnaike***

4:27 Paper 430e: Process Operability Analysis of High-Dimensional Systems
— Jayanth Mondi, Abhishek Baikadi, ***Sivakumar Subramanian***

4:45 Paper 430f: Study of Moment-Based MPC Formulations and Their Connection to Classical Control
— ***Leyla Özkan****, Rongkai Zhang*

5:03 Paper 430g: New Directions on Process Operability: Bilevel and Parallel Programming Approaches for Process Intensification and Modularity
— Juan C. Carrasco, David R. Vinson, ***Fernando V. Lima***

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(431) In Honor of Marco Satyro II (Invited Talks)
Tuesday, Oct 31, 3:15 PM
MCC, L100I
Paul M. Mathias, Chair
John M. Shaw, Co-Chair
Walter Chapman, Co-Chair

Sponsored by:
Thermodynamics and Transport Properties

3:15 Paper 431a: Design Insights for a Thermal Visbreaking Pilot Based on Microwave Heating
— ***Shawn D. Taylor****, Simon Andersen, Tracy Neitz, David O'Brien, Amin Saeedfar, Merlyn Pulikkathara, Wai-Ming Tam*

3:40 Paper 431b: On Cubic EOS Interaction Parameter Estimation for Long Chain n-Alkane + Aromatic Binary Mixtures *—* ***Sourabh Ahitan****, Miao Luo, John B. McLaughlin, John M. Shaw*

4:05 Paper 431c: Uncertainty in Heat Exchanger Design for Diluted Bitumen
— ***Harry Z. Ha****, Paul M. Mathias*

4:30 Paper 431d: *Practical Aspects in Using Distillation VLE and Enthalpy Model*s *—* ***Daniel R. Summers****, Senthil Krishnamoorthy*

4:55 Paper 431e: Bubble Pressure Measurement and Prediction for n-Alkane + Naphthenic Hydrocarbon Binary Mixtures *—* ***Sourabh Ahitan****, John M. Shaw*

5:20 Paper 431f: When Is It Appropriate to Kiss? A Case Study on the Adverse Consequences of Overfitting GE Models
— ***Paul M. Mathias***

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(432) Innovation from Beginning to End: Generating Ideas, Working with People, and Managing Projects
Tuesday, Oct 31, 3:15 PM
MCC, L100G
Eldon Larsen, Chair
Jack Hipple, Co-Chair

Sponsored by: Management Division

3:15 Paper 432a: Innovation from Beginning to End: Generating Ideas, Working with People, and Managing Projects *—* ***Jack Hipple****, Eldon Larsen*

(433) Invited Symposium: Nature-Inspired Electrochemical Systems
Tuesday, Oct 31, 3:15 PM
MCC, M100C
Marc-Olivier Coppens, Chair
Panagiotis Trogadas, Co-Chair
Vijay Ramani, Co-Chair

Sponsored by:
Electrochemical Fundamentals

3:15 Paper 433a: Photochemical Reduction of Enzymes for Light-Driven Chemical Reactions *—* ***Paul King***

3:45 Paper 433b: Using Molecular Catalysts with an Outer Coordination Sphere to Improve Functional Behavior
— ***Wendy Shaw***

4:15 Paper 433c: Termite-Inspired Electrochemical Processing of Lignocellulose to Chemicals and Fuels
— Xiong Peng, Ying Liu, Andrea Kadilak, Sujan Shrestha, Leslie M. Shor, ***William E. Mustain***

4:45 Paper 433d: Nature-Inspired Flow Fields for PEM Fuel Cells
— ***Jason Cho****, Tobias P. Neville, Panagiotis Trogadas, Billy Wu, Dan Brett, Marc-Olivier Coppens*

5:15 Paper 433e: Modeling of Nature-Inspired Hierarchical Porous Materials for Energy Storage
— ***Mostafa Elabyouki****, Maryam Khaleel, Lourdes F. Vega*

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(434) Lignin for Sustainable Industrial Uses
Tuesday, Oct 31, 3:15 PM
MCC, 200B
Amar K. Mohanty, Chair
Manju Misra, Co-Chair

Sponsored by:
Forest and Plant Bioproducts Division

3:15 Introductory Remarks

3:17 Paper 434a: Aromatic Ring Opening of Lignin for Fuel and Chemical Production *—* ***Ruoshui Ma****, Xiao Zhang*

3:42 Paper 434b: Aqueous Lignin Purification with Hot Acids: Cleaning, Fractionating, and Solvating Lignin for Materials Applications
— ***Junhuan Ding****, Adam S. Klett, Jing Jin, Amod A. Ogale, Mark C. Thies*

4:07 Paper 434c: Selectively Cleaving Carbon–Carbon Interunit Linkages in Lignins to Boost Monomer Production
— ***Li Shuai****, Dionisios G. Vlachos, Basudeb Saha*

4:32 Paper 434d: Lignin Value Prior to Pulping: Analyzing Feasibility
— ***Thomas T. Kwok,*** *Hannah E. Santillo, David N. Fogg Jr., Jesse Kautto, Valerie Thomas, Christopher O. Luettgen, Matthew J. Realff, Andreas S. Bommarius*

4:57 Paper 434e: Fractionation of Kraft Lignin by Solvent Extraction and Exploration for Their Value-Added Applications *—* ***Hao Li****, Chunli Li, Lifang Chang*

5:22 Concluding Remarks

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(435) Mathematical Modeling of Transport Processes
Tuesday, Oct 31, 3:15 PM
MCC, M100D
Norman Loney, Chair
Sara Hashmi, Co-Chair

Sponsored by: Transport Processes

3:15 Paper 435a: Numerical Analysis of the Flow, Transport, and Interfacial Phenomena Associated with Growth of Crystalline CZT Under Crucible Rotation
— ***Mia S. Divecha****, Jeffrey J. Derby*

3:30 Paper 435b: Modeling the Transient Shear Flow and Predicting Large-Amplitude Oscillatory Shear (LAOS) Flow of a Thermoreversible Gel Using a Scalar Structure Parameter Thixotropic Model
— ***Matthew Armstrong****, Ryan P. Murphy, Norman J. Wagner, Antony N. Beris*

3:45 Paper 435c: Modeling and Uncertainty Quantification of Vapor Diffusion and Reactions in Polymer
— ***Yunwei Sun****, Hom Sharma, Elizabeth Glascoe*

4:00 Paper 435d: One- and Two-Equation Models to Simulate the Capacitive Deionization Process
— ***Jorge Gabitto****, Costas Tsouris*

4:15 Paper 435e: Modeling of Transport and Reaction in a Novel Hydride Vapor-Phase Epitaxy System
— ***Min Yao****, James B. Rawlings, Thomas F. Kuech*

4:30 Paper 435f: Discretized Modeling of a Simple Motionless 3D Printer Based on Retarded Bending Motion and Electrically Controlled Patterning of Fiber Deposition
— ***Mounica Jyothi Divvela****, Yong L. Joo*

4:45 Paper 435g: A Forward Modeling Approach for the Inverse Estimation of Transient Local Heat Fluxes
— ***Jiu Luo****, Ya-Qiao Wang, Jia-Li Luo, Dong-Chuan Mo, Yuan-Xiang Fu, Shu-Shen Lyu,* ***Yi Heng****, Hiroyuki Ozoe*

5:00 Paper 435h: Modeling of the Evaporation of the Polymer Slurry in the Porous Media *—* ***Shuji Hironaka****, Gen Inoue, Jun Fukai, Yoshifumi Tsuge*

5:15 Paper 435i: Flow of a Power-Law Fluid Across an Asymmetrically Confined Rotating Cylinder
— ***Pooja Thakur,*** *Naveen Tiwari, R. P. Chhabra*

5:30 Paper 435j: Binary Gas Mixture in a High-Speed Channel
— ***Sahadev Pradhan***

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(436) Microreaction Engineering
Tuesday, Oct 31, 3:15 PM
MCC, L100B
Simon Kuhn, Chair
Kishori Deshpande, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

3:15 Paper 436a: Influence of Bubble Growth at the Catalytic Surface on Heat and Mass Transfer in Gas-Liquid-Solid Microreactors *—* ***R. M. Ripken****, J. A. Wood, J. G. E. Gardeniers, S. Le Gac*

3:35 Paper 436b: Anomalous Behavior of Liquid-Liquid Two-Phase Reaction in a Slug-Flow Microreactor *—* ***Anil Vir****, S. Pushpavanam*

3:55 Paper 436c: Toward Fischer-Tropsch Technology Process in Microreactor *—* ***Yousef Alanazi****, Andrew Traverso, Justin Pommerenck, Liney Arnadottir, Alexandre Yokochi, Goran Jovanovic*

4:15 Paper 436d: Motion Tracking of Liquid-Liquid Segmented Flows in Microfluidics and Application to the Briggs-Rauscher Oscillating Reaction
— Daniel Luci, ***Ryan L. Hartman***

4:35 Paper 436e: Highly Controlled Material Transfer into Microfluidic Droplets from an Active Colloidal Continuous Phase *—* ***Tonghan Gu****, Saif A. Khan, T. Alan Hatton*

4:55 Paper 436f: Highly Efficient Synthesis of Polyvinyl Butyral (PVB) Using Microreactor Systems and Recycling Technology
— ***Kai Wang****, Xiyan Lin, Baiyang Zhou,* ***Guangsheng Luo***

5:15 Paper 436g: Commercial 3D-Printed Microreactor for Chemical Analysis *—* ***Andrew Jones***

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(437) Modeling & Simulation of Complex Systems
Tuesday, Oct 31, 3:15 PM
MCC, 103A
Wendy Young, Chair
Jerry Kaczur, Co-Chair

Sponsored by: Innovations of Green Process Engineering for Sustainable Energy and Environment

3:15 Introductory Remarks

3:18 Paper 437a: Optimal Design of Renewable Energy Systems with Flexible Inputs and Outputs by the P-Graph Framework
— Adrian Szlama, Istvan Heckl, ***Heriberto Cabezas***

3:42 Paper 437b: Discovering Heuristics for Sustainable Design by Multiobjective Evolutionary Optimization and Machine Learning
— ***Xinyu Liu****, Bhavik R. Bakshi*

4:06 Paper 437c: Life-Cycle Modeling and Reactor Design for CO_2 Utilization
— Shaik Afzal, Mohamedsufiyan Challiwala, ***Debalina Sengupta****, Nimir Elbashir, Mahmoud El-Halwagi*

4:30 Paper 437d: Methanol Synthesis Using Captured CO_2: Techno-Economic & Environmental Assessment
— ***Jan Schoneberger****, David Hill, Wendy Young*

4:54 Paper 437e: A CFD-Based Dynamic Model of Absorption/Adsorption Process to Simultaneously Purify Landfill Gas and Treat Leachate
— Hecham Omar, ***Sohrab Rohani***

5:18 Paper 437f: Modeling Methods for Concentrating a Formic Acid Product Generated from a Novel Electrochemical Reduction of CO_2 Cell Design *—* ***Jerry Kaczur****, Hongzhou Yang, Syed Dawar Sajjad, Richard I. Masel*

5:42 Concluding Remarks

An up-to-date program is available at www.aiche.org/annual or on the Annual Meeting app
Please refrain from photographing slides or taking video of sessions and presentations.

(438) Multivariate Modeling and Quality-by-Control Approaches for Pharmaceutical Processes
Tuesday, Oct 31, 3:15 PM
MCC, 205A/B

Jacob Albrecht, Chair
Kevin Seibert, Co-Chair

Sponsored by:
Pharmaceutical Discovery, Development and Manufacturing Forum

3:15 Paper 438a: A Method to Reduce Dimensionality of Powder Flow Characterization — ***Yifan Wang***, *Kushal Dhinoja, Fernando J. Muzzio, Celia N. Cruz*

3:37 Paper 438b: Using Mechanistic Modeling of Chromatography to Increase Process Understanding — ***Tim Fattor***, *Stephen Hunt, Jonathan Rocher, Robert Todd*

3:59 Paper 438c: Multivariate Monitoring of a Continuous Manufacturing Process for API Synthesis: Enhancing the Power of Real-Time Data — ***Melanie Dumarey***, *Martin Hermanto*

4:21 Paper 438d: Global System Analysis of Interconnected Flowsheet Models for Drug Product Manufacturing to Performance — ***Pankaj Doshi***, *Marta Moreno Benito, Conrad Davies*

4:43 Paper 438e: Closed-Loop Dynamics of Ribbon Density in a Dry Granulation Process — ***Sudarshan Ganesh***, *Mariana Moreno, Qinglin Su, Zoltan K. Nagy, G. V. Reklaitis*

5:05 Paper 438f: Integrated Control and Data Management System for Continuous Pharmaceutical Manufacturing Process — ***Ravendra Singh***, *Fernando J. Muzzio, Marianthi Ierapetritou, Rohit Ramachandran*

5:27 Paper 438g: In-Silico Process Characterization of Drug Product Filling Operations: Predicting Quality Attributes from First Principles — ***Will Johnson***, *Pablo Rolandi*

(439) Nanoelectronic and Photonic Materials II: 2D Materials
Tuesday, Oct 31, 3:15 PM
MCC, 211A

Pabitra Choudhury, Chair
Subramanian Sankaranarayanan, Co-Chair
Sanchari Chowdhury, Co-Chair

Sponsored by:
Electronics and Photonics

3:15 Paper 439a: Chiral Metamaterial Platform with Tunable Near- and Far-Field Chiroptical Response — ***Pavlos Pachidis***, *Vivian E. Ferry*

3:31 Paper 439b: Lateral Growth of Two-Dimensional 1H-WSe_2/1T'-WTe_2 Heterostructures — ***Mengqiang Zhao***, *Carl H. Naylor, Zhaoli Gao, William M. Parkin, A. T. Charlie Johnson*

3:47 Paper 439c: Nanostructured Optoelectronics Using Interfacially Driven Assembly — ***Matthew G. Panthani***

4:03 Paper 439d: Tuning the Bandgap of Graphene Nanoribbons Through Defect-Interaction-Driven Edge Patterning — ***Dimitrios Maroudas,*** *Lin Du, Andre R. Muniz*

4:19 Paper 439e: Wrinkled MoS2 Field-Effect Transistors — *Shikai Deng,* ***Vikas Berry***

4:35 Paper 439f: Nanoantenna-Enhanced Wavelength Mixing in Monolayer Transition Metal Dichalcogenide — ***D. Keith Roper***, *Gregory T. Forcherio, Mourad Benamara, Luigi Bonacina*

4:51 Paper 439g: Kinetics of Nanoring Formation from Quantum Dots in Epitaxial Thin Films — ***Lin Du***, *Dimitrios Maroudas*

(440) Nanomaterials for Light Harvesting and Novel Photophysical Phenomenon I
Tuesday, Oct 31, 3:15 PM
MCC, 200G

Sang Eon Han, Chair
William A. Tisdale, Co-Chair
Ayaskanta Sahu, Co-Chair

Sponsored by:
Nanomaterials for Applications in Energy and Biology

3:15 Paper 440a: Designing Light-Propelling Nanomotors — ***Jinyao Tang***

3:35 Paper 440b: Improving Electron Transport in TiO_2 Electrode via Nanostructure Engineering — ***Bin Liu***

3:55 Paper 440c: Silicon-Based Infrared Photodetectors Enabled by Hot Electrons — *Seok Jun Han,* ***Sang Eon Han***

4:15 Paper 440d: Enhancing Light Absorption and Emission in Quantum Dot Solids Using Al Nanostructures — ***Matthew K. Quan***, *Vivian E. Ferry*

4:35 Paper 440e: Precise Control over the Morphology and Dopant Distribution in Colloidal Metal Oxide Nanocrystals — ***Ajay Singh***, *Delia J. Milliron*

4:55 Break

(441) Nanoscale Phenomena in Macromolecular Systems
Tuesday, Oct 31, 3:15 PM
MCC, 211C

Jonathan K. Whitmer, Chair
Blair Kathryn Brettmann, Co-Chair

Sponsored by: Polymers

3:15 Paper 441a: Design, Synthesis, and Characterization of Elastomeric and Mechanoresponsive Polymer Matrix Composites — ***Matthew D. Green***

3:45 Paper 441b: Molecular Simulation of Macromolecular Transport Through Nanoporous Membranes — ***Noelia Almodovar Arbelo***, *Bryan W. Boudouris, David S. Corti*

4:00 Paper 441c: Unconventional Nanoscopic Shape Memory Effects Exhibited by Novel Multi-Stimuli-Responsive Shape Memory Polymers — ***Sin-Yen Leo***, *Peng Jiang*

4:15 Paper 441d: Direct Observation of Remarkable Nanostructure Evolution During Aqueous Dissolution of Polymer/Drug Blends — ***Ralm Ricarte***, *Marc A. Hillmyer, Timothy P. Lodge*

4:30 Paper 441e: Effect of Graphene and Graphene Oxide on the LCST of PNIPAM — ***Carter Berry***, *Sanket A. Deshmukh*

4:45 Paper 441f: Solvent Effects on the Structure and Thermodynamics of Polymer Blends with Varying Architectures — ***Thomas Gartner III***, *Arthi Jayaraman*

5:00 Paper 441g: Molecular Weight Dependence of the Intrinsic Size Effect on T_g in AAO Template-Supported Polymer Nanorods: A DSC Study — ***Tong Wei***, *Shadid Askar, Anthony Tan, John M. Torkelson*

5:15 Paper 441h: Versatile Cholesterol-Functionalized Block Copolymers in Aqueous Dispersions — ***Kenneth Mineart***, *Shrinivas Venkataraman, Yi Yan Yang, James L. Hedrick, Vivek M. Prabhu*

5:30 Paper 441i: Polymerization Thermodynamics Under Nanoconfinement — ***Haoyu Zhao***, *Qian Tian, Sindee L. Simon*

(442) Panel Discussion: Rethinking Grand Challenges in Sustainability for the 21st Century (Invited Talks)
Tuesday, Oct 31, 3:15 PM
MCC, 101C

Raymond L. Smith, Chair
Alexander Orlov, Co-Chair

Sponsored by: General

3:15 Paper 442a: Grand Challenges in Sustainability for Future Energy and Chemicals — ***Joseph B. Powell***

3:30 Paper 442b: Research Trends in Sustainable Chemistry and Engineering: Quantifying Progress Toward Sustainability — ***David T. Allen***

3:45 Paper 442c: Hydrogen Economy via Cost-Effective Renewable Solar Water Splitting — ***Alan W. Weimer***

4:00 Paper 442d: Opportunities and Challenges Along the Path to Sustainability — ***Phillip E. Savage***

4:15 Paper 442e: Rethinking Grand Challenges: Panel Discussion — ***Joseph B. Powell***, *David T. Allen, Alan W. Weimer, Phillip E. Savage*

(443) Particle Engineering and Design for Product Value Enhancement
Tuesday, Oct 31, 3:15 PM
MCC, 200H

Ecevit Bilgili, Chair
Ilgaz Akseli, Co-Chair

Sponsored by:
Particle Production and Characterization

3:15 Paper 443a: Dry Mechanical Processing for Value-Enhanced Excipients — *Liang Chen, Xiaoyi Ding, Siqi Fan,* ***Rajesh N. Dave***

3:36 Paper 443b: Assessing the Impact of Dry Coating on the Surface Properties of Pharmaceutical Formulations — ***Eftychios Hadjittofis***, *Geoff G. Z. Zhang, Jerry Heng*

3:57 Paper 443c: Critical Material Attributes (CMAs) of Strip Films Loaded with Poorly Water-Soluble Drug Particles, IV: Surface-Modified Dry Micronized Drug Powders — *Lu Zhang, Yidong Li, Abed Manal,* ***Rajesh N. Dave***

4:18 Paper 443d: Synthesis and Stability Study of Polymorphic Transformed Mannitol/LB Agar Microcarriers for Dry Powder Inhalation — *Fengying Zhang, Thi Quynh Ngoc Nguyen,* ***Raymond Lau***

4:39 Paper 443e: Understanding the Surface Chemistry, Surface Roughness and Wettability of Argon Plasma-Treated Cornstarch Powder — ***Deepa Dixit***, *Shreya Bunk, Ramkrishna Rane, Chinmay Ghoroi*

5:00 Paper 443f: Effects of Baffle Configuration and Tank Size on Spherical Agglomerates of Dimethyl Fumarate in a Common Stirred Tank — ***Tu Lee***, *Po-Yen Lin, Hung-Lin Lee, Chih-Wei Chen*

5:21 Paper 443g: Using Magnetically Assisted Impact Coating (MAIC) for Optimization of Powder Flow Characteristics — ***Charles R. Bowman***, *Tim Freeman, William A. Hendrickson, Christopher J. Rueb, Robert G. Bowman, Katrina Brockbank, Jamie Clayton, Christine M. Colby*

(444) Particulate and Multiphase Flows: Dynamics of Emulsions, Bubbles, Droplets
Tuesday, Oct 31, 3:15 PM
Hilton, Conrad D

Ali Mohraz, Chair
Lilian Hsiao, Co-Chair

Sponsored by: Fluid Mechanics

3:15 Paper 444a: The Shape Evolution of Pendant Droplets in Miscible Environments — ***Dan Walls***, *Simon Haward, Amy Shen, Gerald G. Fuller*

3:30 Paper 444b: Shape Evolution of Miscible Drops with Arbitrary Viscosity Ratio: Lagrangian-Eulerian Swarms of Stokeslets and Subgrid Resolution — ***Ludwig C. Nitsche***, *Paola Leon Plata, Rafael G. Henríquez Rivera, Ying Liu*

3:45 Paper 444c: Coalescence of Drops Due to a Constant-Force Interaction in a Viscous Quiescent Fluid — ***John M. Frostad***, *Alexandra Paul, L. Gary Leal*

4:00 Paper 444d: Dynamics of Viscous Droplets Falling Towards a Micro-Patterned Substrate — ***Yechun Wang***, *Kevin Beussman*

4:15 Paper 444e: Nanoemulsion Formation: Controlling and Predicting Droplet Size — ***Ankur Gupta***, *T. Alan Hatton, Patrick S. Doyle*

4:30 Paper 444f: Using a Novel Approach to Model Drop Size Distribution: The Adaptive Multi-Size Group Method — ***Thomas Eppinger***, *Koichi Akano, Simon Lo, Alexander Vichansky, Ravindra Aglave*

4:45 Paper 444g: Describing Emulsions in Terms of Pseudo-Potential Lattice Boltzmann Modeling — *Mohammad Pourtousi, Siddhartha Mukherjee, Pieter Berghout, Orest Shardt,* ***Harry E. A. Van den Akker***

5:00 Paper 444h: Comparison of the Rise Dynamics of Standard Bubbles and Oil-Coated Bubbles: Experiments and Simulations — ***Songcheng Wang***, *Manoj Kumar Tripathi, Kirti Chandra Sahu, J. Carson Meredith, Sven H. Behrens*

5:15 Paper 444i: Bubble Emergence Through a Packed-Bed Column — ***Mahsa Taghavi***, *Paul Salgi, Vemuri Balakotaiah*

5:30 Paper 444j: A Quadrature-Based Model for Polydisperse Laminar Bubbly Flows — *Jeffrey C. Heylmun, Bo Kong,* ***Alberto Passalacqua***, *Rodney O. Fox*

(445) Phase Behavior, Rheology, and Processing of Nanoparticle Suspensions and Solutions
Tuesday, Oct 31, 3:15 PM
MCC, 213A/B

Matteo Pasquali, Chair
Micah Green, Co-Chair
Anson Ma, Co-Chair

Sponsored by:
Nanoscale Science and Engineering Forum

3:15 Paper 445a: The Microstructure and Rheology of Gels Consisting of Heteroaggregated Nanoparticles — ***Javen Weston***, *Kathleen Weigandt*

3:33 Paper 445b: Direct-Write Fabrication of Nanoparticle Suspensions for High-Density Interconnects — ***Alan Shen***, *Anson W. K. Ma, Sameh Dardona*

3:51 Paper 445c: Interfacial Behavior of Surfactant-Stabilized Carbon Nanotubes in Oil-Water System — ***Tuan V. Vu***, *Dimitrios V. Papavassiliou*

4:09 Paper 445d: Numerical Investigation of Rheological Properties of Nanofluids Containing Organic Modified Nanoparticles — ***Shin Usune***, *Masaki Kubo, Takao Tsukada, Osamu Koike, Rei Tatsumi, Masahiro Fujita, Tadafumi Adschiri*

4:27 Paper 445e: Nanoparticle-Activated and -Directed Assembly of Graphene Nanoscrolls — ***Karteek K. Bejagam***, *Samrendra Singh, Sanket A. Deshmukh*

4:45 Paper 445f: Structured Nanoparticles from the Self-Assembly of Polymer Blends Through Rapid Solvent Exchange — ***Nannan Li***, *Athanassios Z. Panagiotopoulos, Arash Nikoubashman*

5:03 Paper 445g: Effect of Surface Oxidation on the Mechanics of a Carbon Nanotube–Laden Interface — *William D. Ivancic,* ***Christopher L. Wirth***

5:21 Paper 445h: Toward Molecular Engineering of Liquid Crystal Elasticity: Predicting 5CB Elastic Constants — ***Hythem Sidky***, *Jonathan K. Whitmer*

(446) Pyrolysis of Biomass
Tuesday, Oct 31, 3:15 PM
MCC, L100C

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

Sponsored by:
Catalysis and Reaction Engineering Division

3:15 Paper 446a: Mechanistic Modeling of Fast Pyrolysis of Hemicellulose — ***Xiaowei Zhou***, *Wenjun Li, Ross Mabon, Linda J. Broadbelt*

3:37 Paper 446b: Global Kinetics of Species Formation During High-Temperature Pyrolysis of Coal and Biomass in CO_2 Environment — *Aime Tchapda,* ***Sarma Pisupati***

3:59 Paper 446c: Fast-Pyrolysis Kinetic Study for Ten Ecuadorian Agricultural Residual Biomass Samples — ***Diana C. Vargas***, *SriBala Gorugantu, Hans-Heinrich Carstensen, Daniela Almeida Streitwieser, Guy B. Marin, Kevin M. Van Geem*

4:21 Paper 446d: Biomass Pyrolysis: Can a Single Severity Factor Describe the Effect of Pyrolysis Conditions on the Final Biochar Product? — *Lynn Gai,* ***Kyriacos Zygourakis***

4:43 Paper 446e: Real-Time Mass Spectroscopy in Fast-Pyrolysis Process — *Ali Zolghadr,* ***Joseph Biernacki***

5:05 Paper 446f: Measuring the Torrefaction Products of Xylan and D-Xylose — ***Arnab Bose***, *Phillip R. Westmoreland*

5:27 Paper 446g: Agricultural Residue as a Resource for Catalyst Preparation for Bio-Oil Production — ***Shereen Hassan***

(447) Recalcitrance of Woody Biomass
Tuesday, Oct 31, 3:15 PM
MCC, 200E

Subramanian Ramakrishan, Chair
Maobing Tu, Co-Chair

Sponsored by:
Biorefinery Technologies for Forest-Based Lignocellulosic Biomass

3:15 Paper 447a: Stimulation and Inhibition of Organosolv Lignins on Enzymatic Hydrolysis Mediated by Zeta Potential and Hydrophobicity — *Yang Huang,* ***Maobing Tu***, *Thomas Elder*

3:40 Paper 447b: Catalytic Conversion of Corn Stover into Furfural and HMF over Several Carbon-Based Solid Acids — ***Tingwei Zhang***, *Wenzhi Li*

4:05 Paper 447c: Novel Inverse Isotope Effect for Cellulase Hydrolysis of Deuterated Switchgrass — ***Samarthya Bhagia***, *Xianzhi Meng, John Dunlap, Barbara R. Evans, Garima Bali, Jihua Chen, Kimberly S. Reeves, Hoi Chun Ho, Brian H. Davison, Arthur J. Ragauskas*

4:30 Paper 447d: Synthesis of High–Biomass Content UV-Curable Epoxy Acrylate Oligomer with Cardanol — *Zhe Ma,* ***Hao Pang***, ***Bing Liao***, *Yuliang Mai, Wu Wen, Lei Zhang, Yongqiang Dai, Min Gao*

4:55 Paper 447e: Dissolution of Cellulosic Particles: Population Ensemble Modeling Informs Efficient Woody Biomass Processing — *Mohammad Ghasemi, Marina Tsianou,* ***Paschalis Alexandridis***

5:20 Paper 447f: 5-Ethoxymethylfurfural Production from Cellulose Catalyzed by Ultra-Low-Mass-Concentration Sulfuric Acid in One-Pot Reaction — ***Guizhuan Xu***, *Youzhou Jiao, Xuehua Zhou*

(448) Software Tools and Implementations for Process Systems Engineering
Tuesday, Oct 31, 3:15 PM
MCC, 103E

Ruth Misener, Chair
John Siirola, Co-Chair

Sponsored by:
Computing Systems and Technology Division

3:15 Paper 448a: Easy Advanced Global Optimization (EAGO): An Open-Source Platform for Robust and Global Optimization in Julia — ***Matthew Wilhelm***, *Matthew D. Stuber*

3:36 Paper 448b: Proto: Platform for Robust Optimization — ***Logan R. Matthews***, *Yannis A. Guzman, Christodoulos A. Floudas*

3:57 Paper 448c: Recent Developments in Pyomo — ***John D. Siirola***, *Bethany Nicholson, Carl D. Laird*

4:18 Paper 448d: Semantic Repository for Biorefining Model Integration — ***Edlira Kalemi***, *Linsey Koo, Franjo Cecelja*

4:39 Paper 448e: Programmable Process Structures, Generated from a Network and from Functional Meta-Prototypes — ***Monika Varga***, *Bela Csukas*

5:00 Paper 448f: Pyosyn: A Python Tool for General Process Synthesis — ***Qi Chen***, *Anthony P. Burgard, John Eslick, Andrew Lee, John Siirola, David C. Miller, Ignacio E. Grossmann*

5:21 Paper 448g: Super-O: A Tool for Processing Network Synthesis Using Superstructure Optimization — ***Maria-Ona Bertran***, *Lei Zhang, Rafiqul Gani*

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(449) Symposium on Solar Power and Chemical Systems in Honor of Prof. Edward A. Fletcher III

Tuesday, Oct 31, 3:15 PM
MCC, 201A/B

Alexandre Yokochi, Chair
Peter Kreider, Co-Chair
Konstantinos E. Kakosimos, Co-Chair

Sponsored by:
Symposium on Solar Power and Chemical Systems in Honor of Prof. Edward A. Fletcher

3:15 Paper 449a: Keynote — Growing Scientific Leaders from Concentrated Sunlight: A Tribute to Professor E. A. Fletcher — ***Robert Palumbo***, ***Luke Venstrom***

3:45 Paper 449b: Metal Oxide Redox Materials for Solar Thermochemical Energy Storage — *Hossein Beidaghy Dizaji*, ***Peter Kreider***, *Vincent Wheeler, Wojciech Lipinski*

4:05 Paper 449c: SolPeD: Solar per Demand for Power Generation and Fuel Production — ***Jacob Karni***

4:25 Paper 449d: On the Role of Thermochemical Energy Storage in Concentrating Solar Power — *Xinyue Peng, Thatcher W. Root,* ***Christos T. Maravelias***

4:45 Paper 449e: Combined Thermochemical and Latent Heat Energy Storage for Low-Temperature Residential Applications — ***Griffin S. Drake***, *Nick AuYeung*

5:05 Paper 449f: Optical Losses from Bubble Evolution in Photo-Electrochemical Reactors — ***Isaac Gentle***, *Klaus Hellgardt*

5:25 Paper 449g: Laudatio in Honor of Prof. Edward A. Fletcher

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(450) Syngas Production and Gas-to-Liquids Technology

Tuesday, Oct 31, 3:15 PM
MCC, L100F

Erdem Sasmaz, Chair
Hema Ramsurn, Co-Chair
Karthikeyan K. Ramasamy, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

3:15 Paper 450a: Supported Transition Metal Carbides as Catalysts for CO_2 Conversion to Syngas via Reverse Water-Gas Shift Reaction — *Yichen Zhuang, Faisal Mohamed Khan,* ***David Simakov***

3:35 Paper 450b: Molten Salt Chemical-Looping Catalysis for Reactive Separation of HBr in a Halogen-Based Natural Gas-to-Liquids Process — ***D. Chester Upham***, *Zachary Snodgrass, Mojgan Zavareh, Michael Gordon, Horia Metiu, Eric W. McFarland*

3:55 Paper 450c: Development of a Graphene-Supported Iron Oxide Nanocatalyst for Fischer-Tropsch Synthesis — ***Stephen Montgomery***

4:15 Paper 450d: Investigation of a New Preparation Method for Cobalt Fischer-Tropsch Catalysts — ***Mahmood Rahmati***, *Morris D. Argyle, William Hecker, Calvin H. Bartholomew, Mohammad-Saeed Safdari*

4:35 Paper 450e: Short-Chain Hydrocarbons Growth Probability in Fischer-Tropsch Synthesis over Cobalt Catalyst — ***Adolph Muleja***, *Joshua Gorimbo, Yali Yao, Xiaojun Lu, Xinying Liu, Diane Hildebrandt, David Glasser*

4:55 Paper 450f: 2-D Modeling of Fischer-Tropsch Packed-Bed Reactor: First Step Towards Scale-Up — ***Mohamed Sufiyan Challiwala***, *Benjamin Wilhite, Mohammed Minhaj Ghouri, Nimir Elbashir*

5:15 Paper 450g: Heat Generation and Removal in Fixed-Bed Reactors for Fischer-Tropsch Synthesis — *Branislav Todic, Milos Mandic, Nikola Nikacevic,* ***Dragomir B. Bukur***

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(451) Nexus Forum — Options for Addressing Complex, Interconnected Systems

Tuesday, Oct 31, 3:15 PM
MCC, 102A

Dale Keairns, Chair

Sponsored by:
The Food-Energy-Water Nexus

3:15 Panel Discussion

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(452) The Use of CFD in Simulation of Multiphase Mixing Processes

Tuesday, Oct 31, 3:15 PM
MCC, 102D

De-Wei Yin, Chair
Joerg Theuerkauf, Co-Chair

Sponsored by:
North American Mixing Forum

3:15 Paper 452a: Modelling the Separation of Oil and Water in Pipelines — ***Kuochen Tsai***

3:36 Paper 452b: Modeling Pigment Deagglomeration for Industrial Coatings Production — ***Johnathan T. Gorke***, *John Thomas, Bradon J. Dreyer, Jeremy Patt, Alyssa Krutzig, Benjamin Bangasser, Daniel Caron*

3:57 Paper 452c: Investigation of Bubble-Induced Turbulence Model by Direct Numerical Simulation — ***Xin Feng***, *Chao Yang, Zai-Sha Mao, Gretar Tryggvason*

4:18 Paper 452d: CFD Simulation of a Pulse-Jet-Mixed Vessel — ***Jung W. Kim***, *Richard V. Calabrese*

4:39 Paper 452e: CFD-Based Multi-Objective Optimization of Dual-Impeller Configurations in a Gas-Liquid Stirred Tank — ***Jia-Jun Wang***

5:00 Paper 452f: Operating Condition Optimization on Mass Transfer in Aerated Stirred-Tank Fermentors — ***Leonard Becker***, *Ravindra Aglave, Thomas Eppinger*

5:21 Paper 452g: Predicting Temperature Profile of Partially Filled Twin-Screw Extruder Using 3D Multiphase CFD Model — ***Chang Kai Wu***, *Hossam Metwally*

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(453) Thermophysical Properties and Phase Behavior II: Electrolytes and Ionic Liquids

Tuesday, Oct 31, 3:15 PM
MCC, L100J

Jindal K. Shah, Chair
Shuangliang Zhao Sr., Co-Chair
Hiroyuki Matsuda, Co-Chair

Sponsored by:
Thermodynamics and Transport Properties

3:15 Paper 453a: Prediction of Mean Ionic Activity Coefficient of NaCl-H_2O System at High Concentrations Using Molecular Dynamics Simulations — ***Nazir Hossain***, *Ashwin Ravichandran, Rajesh Khare, Chau-Chyun Chen*

3:34 Paper 453b: Thermodynamic Modeling of Lithium Salt Systems with the Electrolyte NRTL Model — ***Toni Kirkes***, *Chau-Chyun Chen*

3:53 Paper 453c: Why Tetrabutylphosphonium Hydroxide–Water Mixtures Can Dissolve Cellulose at Extremely High Water Mass Fractions — *Brad Crawford,* ***Ahmed E. Ismail***

4:12 Paper 453d: Phase Behavior of Compressed Gases in Ionic Liquids at the Liquid-Solid Transition Point — ***David L. Minnick***, *Brooks B. Danahy, Mark B. Shiflett*

4:31 Paper 453e: Is Difference in Hydrogen Bond Ability of Anions an Exclusive Descriptor of Nonideality in Binary Ionic Liquid Mixtures? — ***Utkarsh Kapoor***, *Jindal K. Shah*

4:50 Paper 453f: Polymer–Solvent Phase Behavior of Lignin with Hot Aqueous Solvent Systems — ***Junhuan Ding***, *Adam S. Klett, Jordan A. Gamble, Graham W. Tindall, Mark C. Thies, Mark E. Roberts*

5:09 Paper 453g: Application of Thermodynamic Models in the Context of Liquid Chromatography — ***Franziska Ortner***, *Chantal Ruppli, Marco Mazzotti*

5:28 Paper 453h: The Solubility and the Freezing Point Depression (FPD) Measurements of Na-1-Ethanethiolate, Na-1-Propanethiolate, Na-2-Propanethiolate, Na-1-Butanethiolate and Na-2-Methyl-2-Propanethiolate Salts in Pure Water — ***Javeed Awan***

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(454) Unconventional Technologies for CO_2 Capture, Conversion and Utilization

Tuesday, Oct 31, 3:15 PM
MCC, 103B

Kriston Brooks, Chair
Wei Liu, Co-Chair
Xiangping Zhang, Co-Chair

Sponsored by:
Innovations of Green Process Engineering for Sustainable Energy and Environment

3:15 Paper 454a: Carbon Dioxide Utilization in Geothermal Power Generation and Geologic Energy Storage — ***Jimmy Randolph***, *Thomas A. Buscheck, John Griffin, Martin Saar*

3:35 Paper 454b: Efficiency Limits of an Integrated Solar-Driven CO_2 Capture and Reduction System — ***Aditya Prajapati***, *Meenesh R. Singh*

3:55 Paper 454c: A Process Integration Approach for a Sustainable GTL Process Using Tri-Reforming of Methane — ***Mohamed Sufiyan Challiwala***, *Debalina Sengupta, Mahmoud El-Halwagi, Nimir Elbashir*

4:15 Paper 454d: Ozonolysis in Liquid CO_2 as a Platform for Processing of Distributed Feedstocks — ***Michael D. Lundin***, *Andrew Danby, Xuhui Chen, Bala Subramaniam*

4:35 Paper 454e: Understanding the Effects of Carbon Dioxide and Bicarbonate on Chlamydomonas reinhardtii — ***Humeyra B. Ulusoy Erol***, *Jamie A. Hestekin, Christa N. Hestekin, Yupo J. Lin, Benjamin Drewry, Catherine Atchley*

4:55 Paper 454f: Power-to-Gas: Dynamic Modeling of a Catalytic Methanation Reactor — ***Axel Fache***, *Frédéric Marias, Vincent Guerré, Stéphane Palmade*

5:15 Paper 454g: The Effect of Water on CO_2 Capture by AHA Ionic Liquids — ***Gabriela Avelar***, *Oscar Morales, Joan F. Brennecke*

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(455) Value-Added Co-Products from Biorefineries

Tuesday, Oct 31, 3:15 PM
MCC, 101B

Blake Simmons, Chair
Ana I. Torres, Co-Chair

Sponsored by:
Sustainable Biorefineries

3:15 Paper 455a: Acrylonitrile Production from Biomass-Derived Intermediates — ***Gregg T. Beckham***, *Mary Biddy, Adam Bratis, Todd Eaton, Eric M. Karp, Violeta Sànchez i Nogué, Derek Vardon*

3:40 Paper 455b: Multistream Integrated Biorefinery (MIBR) for Carbon-, Road-, and Bio-Materials — *Shangxian Xie, Qiang Li,* ***Joshua Yuan***

4:05 Paper 455c: Improving Economics of Cellulosic Biofuels: An Integrated Strategy for Co-Producing 1,5-Pentanediol and Bioethanol — ***Kefeng Huang***, *Wangyun Won, Zachary Brentzel, Kevin J. Barnett, David Martin Alonso, James A. Dumesic, George W. Huber, Christos T. Maravelias*

4:30 Paper 455d: High-Value Products from a Photobioreactor-Based Biorefinery — ***Ronald R. Chance***, *Yanhui Yuan, Teresa Fishbeck, Harlan Miller, William Porubsky, Imke Lang, Rocco Fiato*

4:55 Paper 455e: A Highly Selective Dehydration of D-Xylose and Wheat Straw C5-Sugars into Furfural by Using Supercritical CO_2 as Catalyst: A Green and Efficient Approach — ***Ana R. C. Morais***, *Rafal M. Lukasik*

5:20 Paper 455f: Process Design for the Synthesis of Biodiesel, Glycerol, 3-Hydroxypropionic Acid and 1,3-Propanediol — ***Tereza Kolaiti***, *Rafiqul Gani, John M. Woodley*

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(456) Plenary Session: AES Electrophoresis Society (Invited Talks)

Tuesday, Oct 31, 3:30 PM
Hilton, Marquette IV/V/VI/VII

Soumya Srivastava, Chair
Tayloria Adams, Co-Chair

Sponsored by:
2017 Annual Meeting of the AES Electrophoresis Society

3:30 Paper 456a: Nanoplasmonic Biosensors: From Innovative Materials to Multimode Sensing with Integrated Microdevices — ***Amy Shen***

4:00 Paper 456b: Novel Consumables for High-Throughput Screening That Capitalize on Electrical Forces and Leverage Existing Laboratory Tools — ***Vincent T. Remcho***

4:30 Paper 456c: Analysis of Single Nucleic Acid Molecules in Micro- and Nano- Fluidics — ***Jeff Wang***

5:00 Paper 456d: New Paradigms in Gel Electrophoresis with Non-Newtonian Fluids — ***Lisa A. Holland***

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(457) SBE's James E. Bailey Award Lecture

Tuesday, Oct 31, 6:00 PM
MCC, Ballroom B

Sponsored by: Awards Committee

6:00 Paper 457a: Biomaterials for Tissue Engineering — ***Antonios G. Mikos***

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(458) Adsorption Applications for Sustainable Energy and Chemicals

Wednesday, Nov 1, 8:00 AM
MCC, M100F

Fateme Rezaei, Chair
F. Handan Tezel, Co-Chair

Sponsored by:
Adsorption and Ion Exchange

8:00 Paper 458a: Sorption of Organic Acids on Weak-Base Anion-Exchange Resins with Different Basicities — ***Haripriya Naidu***, *Alexander P. Mathews*

8:18 Paper 458b: N_2-Selective Cation-Exchanged Clinoptilolite: Adsorption Separation of N_2 from CH_4-Containing Mixtures — ***Dean Kennedy***, *Maja Mujcin, F. Handan Tezel*

8:36 Paper 458c: Fundamentals of Competitive Adsorption Phenomena Within Dilute, Multi-Component Aqueous Mixtures — ***Abdulaziz Alturki***, *Dante Simonetti*

8:54 Paper 458d: Evaluation of Solid Adsorbents as Buffer Materials for Indoor Air CO_2 Control — *Pavithra E. Rajan, Anirudh Krishnamurthy, Glenn Morrison,* ***Fateme Rezaei***

9:12 Paper 458e: Adsorption Models for Treatment of Nuclear Reprocessing Off-Gases — ***Austin Ladshaw***, *Sotira Yiacoumi, Yue Nan, Lawrence L. Tavlarides, Costas Tsouris*

9:30 Paper 458f: Nanostructured Conducting Polymers for Electrochemically Mediated Separations of Organic Pollutants from Water — ***Yinying Ren***, *Xianwen Mao, Zhou Lin, Emily Penn, Troy van Voorhis, T. Alan Hatton*

9:48 Paper 458g: Understanding Gravimetric and Volumetric Hydrogen Cryo-Adsorption Trade-Off in Metal-Organic Frameworks (MOFs) and Its Link to Material Properties — *Grace Anderson, Paula Garcia-Holley, Benjamin Schweitzer, Ryther Anderson, Omar K. Farha, Taner Yildirim,* ***Diego Gomez Gualdron***

10:06 Paper 458h: Modeling of Multicomponent Sorption of Fermentation Products on Resin Sorbents — *Alexander P. Mathews,* ***Haripriya Naidu***

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(459) Advanced Inorganic Materials for Membrane Gas Separation — GS I

Wednesday, Nov 1, 8:00 AM
MCC, M100I

Ali A. Rownaghi, Co-Chair
Bin Mu, Co-Chair
Seok-Jhin Kim, Co-Chair

Sponsored by:
Membrane-Based Separations

8:00 Paper 459a: Pervaporation and Vapor Permeation Separation of Xylene Mixture by Randomly Oriented MFI Zeolite Membranes — ***Jerry Lin***, *Fateme Bamihashemi, Lie Meng*

8:19 Paper 459b: Suppressing Substructure Collapse in Carbon Molecular Sieve (CMS) Hollow Fibers — ***Oishi Sanyal***, *Shweta Karwa, Nitesh Bhuwania, Stephanie Hicks, William Koros*

8:38 Paper 459c: Chabazite SAPO-34 Zeolite Membranes for Krypton/Xenon Separation: Enhanced Separation Performance and Process Modeling — ***Yeon Hye Kwon***, *Christine Kiang, Ramesh Bhave, Sankar Nair*

8:57 Paper 459d: Synthesis of MOF-Based Membranes Through Chemical Vapor Growth — ***Xiaoli Ma***, *Dandan Xu, Michael Tsapatsis*

9:16 Paper 459e: Zeolitic-Imidazolate Framework ZIF-8 Membranes on Ceramic Tubular Supports for Scalable High-Resolution Propylene/Propane Separation — ***Jingze Sun***, *Hae-kwon Jeong*

9:35 Paper 459f: Gas Mixture Separation Through Nanoporous Graphene Membranes — ***Jesse D. Benck***, *Zhe Yuan, Yannick Eatmon, Michael Strano*

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(460) Advanced Treatment for Water Reuse and Recycling

Wednesday, Nov 1, 8:00 AM
MCC, 102F

Andi Rahardianto, Chair
Jeffrey McCutcheon, Co-Chair
Sage R. Hiibel, Co-Chair

Sponsored by: Water

8:00 Paper 460a: Solar-Driven Electrochemical Desalination of Seawater — ***Emily C. Yolo***, *Aditya Prajapati, Meenesh R. Singh*

8:15 Paper 460b: Salt Harvesting of Reverse-Osmosis Concentrate by Continuous Chemically Enhanced Seeded Precipitation — ***Jin Yong Choi***, *Anditya Rahardianto, Yoram Cohen*

8:30 Paper 460c: 3D Carbon Material and Its Excellent Capacitive Deionization Performance — ***Liang Chang***, *Yun Hang Hu*

8:45 Paper 460d: Nutrient Recovery from Thermally Treated Agriculture Waste Using Membrane Distillation — ***Nicholas Silva***, *Saeed Vahed Qaramaleki, Silvia Román, Charles J. Coronella, Sage R. Hiibel*

9:00 Paper 460e: Investigation of Growth Kinetics of Debaryomyces hansenii in Petroleum Refinery Desalter Effluent — ***Leila Azimian***, *Amarjeet Bassi, Rebecca Rena Elgrichi*

9:15 Paper 460f: Recovery and Reuse of Aluminum in Municipal Wastewater — ***Tulip Chakraborty***, *Michelle Gabriel, Ali Amiri, Domenico Santoro, John Walton, Scott Smith, Madhumita Ray, George Nakhla*

9:30 Paper 460g: First Principles of Metal-Ion Extraction from Non-Buffered Water with Hydrophobic Deep Eutectic Solvents — ***Dannie J. G. P. van Osch***, *Dries Parmentier, Adriaan van den Bruinhorst, Carin H. J. T. Dietz, Remco Tuinier, Maaike C. Kroon*

(461) Advances in Optimization II
Wednesday, Nov 1, 8:00 AM
MCC, 103E

M. M. Faruque Hasan, Chair
Fengqi You, Co-Chair

Sponsored by:
Computers in Operations and Information Processing

8:00 Paper 461a: Robust Optimization with Decision-Dependent Uncertainty Sets — ***Nikolaos Lappas***, *Anirudh Subramanyam, Chrysanthos E. Gounaris*

8:21 Paper 461b: Optimization Under Uncertainty Using Surrogate Models for Confidence Evaluation — *Ronak Pipaliya, Alec Rigsbee,* ***Edward P. Gatzke***

8:42 Paper 461c: Multistage Adaptive Conditional Value at Risk Optimization Using Piecewise Linear Decision Rule — *Said Rahal,* ***Zukui Li***

9:03 Paper 461d: Derivation of Generalized Affine Decision Rules for Mixed-Integer Linear, Quadratic and Nonlinear Adjustable Robust Optimization Problems by Multi-Parametric Programming — ***Styliani Avraamidou***, *Chao Ning, Fengqi You, Efstratios N. Pistikopoulos*

9:24 Paper 461e: A Predictor-Corrector Algorithm for Projection-Based Derivative-Free Optimization — ***Ishan Bajaj***, *M. M. Faruque Hasan*

9:45 Paper 461f: Optimization of Black-Box Problems Using Smolyak Grids and Polynomial Approximations — *Chris A. Kieslich,* ***Fani Boukouvala***

10:06 Paper 461g: On the Impact of Solution Representations for Stochastic Optimisation of Control Trajectories of Industrial Fermentation Processes — ***Alistair D. Rodman***, *Eric S. Fraga, Dimitrios I. Gerogiorgis*

(462) Advances in Process Intensification: Enhanced Reactivity and Separations
Wednesday, Nov 1, 8:00 AM
MCC, 101E

James A. Ritter, Chair

Sponsored by:
Process Intensification & Modular Chemical Processing

8:00 Paper 462a: A General Adsorption/Reaction Framework for Modular and Multi-Functional Process Design — ***Akhil Arora***, *Shachit S. Iyer, M. M. Faruque Hasan*

8:25 Paper 462b: Ultrasonic Tuning of TiO_2-Based Mixed Oxides' Structural Properties and Catalytic Activity — *Marta Stucchi, Amal El Fiad, Claudia Bianchi,* ***Daria C. Boffito***

8:50 Paper 462c: Multi-Model Operability Approach for Process Design, Intensification and Modularity: Application to Nonlinear and High-Dimensional Membrane Reactors — ***Vitor Gazzaneo***, *Juan C. Carrasco, Fernando V. Lima*

9:15 Paper 462d: A Modeling Methodology for Predicting Intensified CO_2 Removal Efficiency with Rotating Packed Bed — ***Cheng-Hsiu Yu***, *Chau-Chyun Chen*

9:40 Paper 462e: Carbon Dioxide Capture by Sodium Hydroxide-Glycerol Aqueous Solution in a Rotating Packed Bed — ***Hwai-Shen Liu***

10:05 Paper 462f: Graphic Synthesis Method for Multi-Technique Integration Separation Sequences of Multitudinous Refinery Gases — ***Xuehua Ruan***, *Hongyan Xiao, Xiaobin Jiang, Xiaoming Yan, Yan Dai, Gaohong He*

(463) Alternative Fuels and Enabling Technologies
Wednesday, Nov 1, 8:00 AM
MCC, 200A

Karthikeyan K. Ramasamy, Chair
Nazmul Karim, Co-Chair

Sponsored by:
Alternate Fuels and New Technology

8:00 Break

8:25 Paper 463b: Evaluation of Aromatics Formation in Thermal Cracking of Triglycerides — *Ramon F. Beims, Laércio Ender, Vanderleia Botton, Dilamara R. Sharf, Edésio L. Simionatto, Henry F. Meier,* ***Vinicyus R. Wiggers***

8:50 Paper 463c: Tuning the Structure and Electronic Properties of Manganese Nitrides for Ammonia Production from First-Principles Modeling — ***Bin Liu***, *Nannan Shan, Peter H. Pfromm*

9:15 Paper 463d: Rapid and Extended Analysis of Syngas Using Micro GC Fusion — ***Shawn Wilson***

9:40 Paper 463e: Modelling Studies for Cavity Growth in Underground Coal Gasification — ***Sreeja Narayanan***, *Preeti Aghalayam*

10:05 Paper 463f: Dual-Alcohol Blending Effects on Gasoline Properties — ***Saeid Aghahossein Shirazi***, *Thomas D. Foust, Kenneth F. Reardon*

(464) Biomolecules at Interfaces I
Wednesday, Nov 1, 8:00 AM
MCC, M100B

Prajnaparamita Dhar, Chair
Susan Daniel, Co-Chair
Bernardo Yanez Soto, Co-Chair

Sponsored by: Interfacial Phenomena

8:00 Welcoming Remarks

8:03 Paper 464a: Computation of Amino Acid-Mineral Surface Thermodynamics and Interaction Modes via Importance Sampling — *Kayvon Tabrizi, Michael S. Pacella,* ***Jeffrey J. Gray***

8:19 Paper 464b: Research on the Mechanism of Spontaneous DNA Extension on Grooved Surface Covered with Cationic Lipid Bilayers — *Tzu-Hsien Fan, Hou-Jun Guo,* ***Chih-Chen Hsieh***

8:35 Paper 464c: Effect of Interchain Associations on Hybridization Activity of DNA Brushes — *Hao-Chun Chiang,* ***Rastislav Levicky***

8:51 Paper 464d: Understanding Marine Mussel Adhesion: Interfacial Energy from Microscopic to Macroscopic Length Scales — ***George Degen***, *Jacob Israelachvili*

9:07 Paper 464e: Tuning Underwater Adhesion with Cation-Pi Interactions — ***Matthew A. Gebbie***, *Jacob N. Israelachvili, J. Herbert Waite*

9:23 Paper 464f: Influence of the Surface Charge on the Brownian Motion of Colloidal Particles near Surfaces with Biomimetic Characteristics — *Juan Manuel Hernandez Meza, Angeles Ramírez-Saíto, B. Jose Luis Arauz-Lara, Said E. Aranda Espinoza,* ***Bernardo Yanez Soto***

9:39 Paper 464g: Charged Nanoparticles Interacting with Giant Vesicles Fabricated from Inverted-Headgroup Lipids — ***Lu Wang***, *Noah Malmstadt*

9:55 Paper 464h: Modulation of Phase Morphology of Surfactant Monolayer with Interfacial Curvature — ***Amit Kumar Sachan***, *Joseph A. Zasadzinski*

10:11 Paper 464i: Recognition of Target Cells by Vibrio cholerae Outer Membrane Vesicles — *Elnaz S. Rasti,* ***Angela C. Brown***

10:27 Concluding Remarks

(465) Catalysis with Microporous and Mesoporous Materials III
Wednesday, Nov 1, 8:00 AM
MCC, L100A

Michele L. Sarazen, Chair
Viktor J. Cybulskis, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

8:00 Paper 465a: Mechanism for Selective Fructose Etherification on Hierarchical Sn-SPP Zeolite — ***Tyler R. Josephson***, *Limin Ren, Qiang Guo, Swagata Pahari, Robert F. DeJaco, Michael Tsapatsis, J. Ilja Siepmann, Dionisios G. Vlachos, Stavros Caratzoulas*

8:18 Paper 465b: Group IV and V Periodic Trends in Olefin Epoxidation: Effects of Local Environment and Electronic Structure — ***Daniel T. Bregante***, *Nicholas E. Thornburg, Justin M. Notestein, David W. Flaherty*

8:36 Paper 465c: Sulfur Deactivation Pathways in Cu-SSZ-13 Determined Through First-Principle Modeling and X-Ray Spectroscopy — ***Hui Li***, *Arthur J. Shih, Ashok Kumar, Juan M. Gonzalez, Ishant Khurana, Christopher Paolucci, Jeffrey Miller, Tianpin Wu, Aleksey Yezerets, Rajamani Gounder, Fabio H. Ribeiro, William F. Schneider*

8:54 Paper 465d: Catalytic Consequences of Framework Polarity for Ethanol Dehydration on Sn-Beta Zeolites — ***Jason S. Bates***, *Brandon C. Bukowski, Jeffrey P. Greeley, Rajamani Gounder*

9:12 Paper 465e: Size-Selective Oxidation of Alkanes by Microporous Oxides — ***Annamalai Leelavathi,*** *Prashant Deshlahra*

9:30 Paper 465f: Impact of Hydrocarbon Trapping on Temperature-Programmed Oxidation over a Pt/Pd/BEA Monolith Catalyst — *Po-Yu Peng,* ***Michael P. Harold***, *Dan Luss*

9:48 Paper 465g: Consequences of Diffusion, Acid Strength, and Confinement on Bifunctional Reactions of Alkanes — ***Gina Noh***, *Enrique Iglesia*

10:06 Paper 465h: Hydrophobic Zeolites for Solketal Production from Crude Glycerol — ***Thanh Khoa Phung***, *Md. Anwar Hossain, Sarttrawut Tulaphol, Teerawit Prasomsri, Noppadon Sathitsuksanoh*

(466) Cell Culture Engineering & Process Design I: Cell Systems Engineering
Wednesday, Nov 1, 8:00 AM
MCC, 208C/D

Kang Zhou, Chair
Nicholas Graham, Co-Chair

Sponsored by: Bioengineering

8:00 Paper 466a: Use of Site-Specific Recombinases to Engineer New Cell Lines for Therapeutic Protein Biomanufacturing — ***Sofie A. O'Brien***, *Christopher Stach, Kyoungho Lee, Meghan G. McCann, Nikunj Somia, Michael J. Smanski, Wei-Shou Hu*

8:18 Paper 466b: Implications of Protein Sequence Variants Derived from Systematic Starvation — ***H. Edward Wong***, *Jack Chung-Jr Huang, Zhongqi Zhang*

8:36 Paper 466c: Anti-Adhesive Glycosylated Proteins as a Technology for Improved Suspension Cell Culture in Bioreactors — ***Shelby Head***, *Carolyn Shurer, Marshall Colville, Vivek Gupta, FuiBoon Kai, Jonathon Lakins, Matthew Paszek, Heidi Reesink*

8:54 Paper 466d: Multi-Omics Approaches to Unravel Cellular Metabolism Towards Enhancing Process Robustness — ***Ravali Raju***, *Amr Ali, Alan Gilbert, Rashmi Kshirsagar*

9:12 Paper 466e: Epigenomic Analysis on Chinese Hamster Ovary (CHO) Cells for Enhanced Production Cell Line Stability — ***Zion Lee***, *Wei-Shou Hu*

9:30 Paper 466f: CRISPR/Cas9-Mediated Knock-In of an Optimized TetO Repeat for Live Cell Imaging of Endogenous Loci — ***Ipek Tasan***, *Liguo Zhang, Gabriela Sustackova, Jiah Kim, Mayandi Sivaguru, Mohammad HamediRad, Yuchuan Wang, Justin Genova, Jian Ma, Andrew Belmont, Huimin Zhao*

9:48 Paper 466g: Continuous Processing Strategies for Biologics Manufacturing — ***Weichang Zhou***

(467) Cellulose-Based Materials
Wednesday, Nov 1, 8:00 AM
MCC, 200E

Yulin Deng, Chair
Junyong Zhu, Co-Chair

Sponsored by:
Forest and Plant Bioproducts Division

8:00 Paper 467a: High-Performance Magnetic-Activated Carbon from Solid Waste from Lignin Conversion Processes, 1: Their Use as Adsorbents for CO_2 — *Wenming Hao,* ***Fredrik Björnerbäck***, *Yulia Trushkina, Mikel O. Bengoechea, German Salazar-Alvarez, Tanja Barth, Niklas Hedin*

8:25 Paper 467b: Surface Structure Patterning for Fabricating Non-Fluorinated Super-Hydrophobic Cellulosic Membrane — ***Wei Liu***, *Xu Du, Zhe Zhang, Yulin Deng*

8:50 Paper 467c: Photonic Cellulose Nanocrystal (CNC) Coatings — ***Partha Saha***, *Virginia A. Davis*

9:15 Paper 467d: Study of Pyrolysis Products of Live and Dead Shrub Fuels from the Forest in the Southeastern United States — ***Mohammad-Saeed Safdari***, *Joel Howarth, Mahmood Rahmati, Thomas H. Fletcher*

9:40 Paper 467e: Electroanalytical Investigations on the Performance of Two-Compartment and Three-Compartment Lignocellulose-Fed Bioelectrochemical Energy Systems — ***Xu Zhang***

10:05 Paper 467f: The Study of the Feasibility of Joint Production of Jet Fuel and Bioethanol from Biomass — ***Xu Zhang***

(468) Complex Fluids: Macromolecules
Wednesday, Nov 1, 8:00 AM
Hilton, Marquette I/II/III/VIII/IX

Simon Rogers, Chair
Subramanian Ramakrishnan, Co-Chair

Sponsored by: Fluid Mechanics

8:00 Paper 468a: Applying Computational Tools of Polymer Field Theory to Out-of-Equilibrium Polymer Solutions in Flow — *Charles Young,* ***Charles E. Sing***

8:30 Paper 468b: Capillary Thinning and Pinch-Off Dynamics and Extensional Rheology of Polyelectrolyte Solutions — *Leidy N. Jimenez, Jelena Dinic, Nikhila Parsi,* ***Vivek Sharma***

8:45 Paper 468c: Relaxation of Knotted Polymers — ***Vivek Narsimhan***, *Alexander Klotz, Patrick S. Doyle*

9:00 Paper 468d: On Synthetic Drilling Fluid Rheological Modelling — ***Silvio Baldino***, *Reza E. Osgouei, Evren Ozbayoglu, Stefan Z. Miska*

9:15 Paper 468e: Experimental Evidence for Shear Banding in Large-Amplitude Oscillatory Shear of Entangled DNA Solution — ***Seunghwan Shin***, *Kevin D. Dorfman, Xiang Cheng*

9:30 Paper 468f: Padé Approximants for Shear Stress in Large-Amplitude Oscillatory Shear Flow — *Chaimongkol Saengow,* ***A. Jeffrey Giacomin***, *Nidal Khalaf, Martin Guay*

9:45 Paper 468g: The Effect of Branching on Shear Band Formation and Evolution in Wormlike Micelles (WLMs) — ***Michelle A. Calabrese***, *Simon A. Rogers, Lionel Porcar, Norman J. Wagner*

10:00 Paper 468h: Predictions for Non-Linear Flows of Polydisperse Blends Based on a Differential-Constitutive Analogue of the Double-Reptation Model — ***Joseph Peterson***, *L. Gary Leal, Glenn H. Fredrickson*

10:15 Paper 468i: Marangoni Instability During the Non-Solvent-Induced Phase Separation of a Ternary Polymer Solution — ***Douglas Tree***, *Glenn H. Fredrickson*

(469) Computational Catalysis II: Metal and Alloy Catalysis
Wednesday, Nov 1, 8:00 AM
MCC, L100E

Giannis Mpourmpakis, Chair
Matthew M. Montemore, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

8:00 Paper 469a: Support Effects in Heterogeneous Catalysis Using Au Nanoparticles on Oxides: A DFT Analysis — ***Paulami Majumdar***, *Yanran Cui, Fabio H. Ribeiro, Jeffrey P. Greeley*

8:18 Paper 469b: Coordination-Based Descriptors for Rational Design of Metal Nanocatalysts — ***Siwen Wang***, *Hongliang Xin*

8:36 Paper 469c: Theoretical Investigation of the Ring Opening Mechanism of Cyclohexanes on Ir Surfaces — ***Kushal Ghale***, *Ye Xu*

8:54 Paper 469d: CO_2 Reduction on the Nickel Surface — ***Wei Lin***, *George C. Schatz*

9:12 Paper 469e: Designing Cu-Based Bimetallic Nanoparticles for CO_2 Activation — ***James Dean***, *Giannis Mpourmpakis*

9:30 Paper 582h: Understanding Heterogeneous Catalyst Deactivation By Biogenic Impurities on Ni (111) Surface and Bimetallic Alloy — ***Madhulika Gupta***, *Tuhin Suvra Khan, Shelaka Gupta, Md. Imteyaz Alam, Manish Agarwal, M. Ali Haider*

9:48 Paper 469g: Determination of Iridium Alloy Properties for Catalytic Applications — ***Lida Mehdizadegan Namin***, *N. Aaron Deskins*

10:06 Paper 469h: Identifying Reaction Pathways for the Sabatier Reaction on Stepped Metal (211) Surfaces — ***Devyani Sharma***, *Karsten Reuter, Mie Andersen*

(470) Computational Methods in Biological and Biomedical Systems II
Wednesday, Nov 1, 8:00 AM
MCC, 103F

Stacey D. Finley, Chair
Nigel Reuel, Co-Chair
Ashlee N. Ford Versypt, Co-Chair

Sponsored by:
Applied Mathematics and Numerical Analysis

8:00 Paper 470a: Seamless Particle-Based Modeling of Blood Clotting — ***Alireza Yazdani***

8:19 Paper 470b: Incorporating Computational Fluid Dynamics into the Study of Cell Damage Due to Hydrodynamic Stress in Bioreactors and Pumps — ***James Kim***

8:38 Paper 470c: A New Patient-Specific Targeted Pulmonary Drug Delivery Method to Treat Lung Cancer Using E-Cigarette Technology — ***Yu Feng***, *Ahmadreza Haghnegahdar, Xiaole Chen, Mingshi Yang*

8:57 Paper 470d: A Computational Fluid Dynamics Analysis of the Carotid Artery — ***David G. Foster***, *Dominick Salerno*

9:16 Paper 470e: CFD-Based Validation of Drug Metabolism from Clinical Data in 3D Configuration — ***Carrie German***, *Sundararajan V. Madihally*

9:35 Paper 470f: On the Numerical Validity of Commonly Employed Scaffold Mimics for Shear Stress and Flow Field Calculations in Tissue Engineering Models — ***Olufemi Kadri***, *Roman Voronov, Vassilios I. Sikavitsas, Cortes Williams III, Robert L. Shambaugh*

9:54 Paper 470g: A Computational Multiphase Flow Model to Predict the Transport and Deposition of Inhaled Flu Virus-Laden Droplets in Human Respiratory Tracts for Early Infection Diagnosis — ***Yu Feng***, *Ahmadreza Haghnegahdar, Xiaole Chen*

10:13 Paper 470h: Optimal Mechano-Electric Treatment of Ventricular Fibrillation — ***Azzam Hazim***, *Youssef Belhamadia, Stevan Dubljevic*

(471) CO_2 Capture, Utilization, and Disposal: Key to Clean Energy Production II

Wednesday, Nov 1, 8:00 AM
MCC, 200F

Sponsored by:
Transport and Energy Processes

8:00 Paper 471a: Transport Analysis of an Integrated Artificial Photosynthetic System for Direct Capture and Reduction of CO_2 from Air
— ***Grzegorz Kokoszka***, *Aditya Prajapati, Meenesh R. Singh*

8:25 Paper 471b: Design of a 400 MW Carbon-Neutral, Coal-Fired Power Plant with Integration of Waste Heat and Solar Energy — ***Rosanna Granata***, *Aditya Prajapati, Meenesh R. Singh*

8:50 Paper 471c: The Energetics of Chemical-Looping Processes for Post-Combustion CO_2 Capture
— ***Hugo S. Caram***, *Fan Ni, Ramesh Gupta, Hans Thomann*

9:15 Paper 471d: A Technoeconomic Evaluation of Carbon Dioxide (CO_2) Electroreduction: Results and Implications — ***Sumit Verma***, *Byoungsu Kim, Molly Jhong, Shawn Lu, Sichao Ma, Paul J. A. Kenis*

9:40 Paper 471e: A Coupled Wellbore-Reservoir Numerical Simulator and Its Integration with Techno-Economic Model GEOPHIRES for Enhanced Geothermal Systems
— ***Manish Nandanwar***, *Brian J. Anderson, Nagasree Garapati*

(472) Crystallization of Pharmaceutical and Biological Molecules

Wednesday, Nov 1, 8:00 AM
MCC, M100J

Ryan C. Snyder, Chair
Venkateswarlu Bhamidi, Co-Chair
Ying Diao, Co-Chair

Sponsored by:
Crystallization and Evaporation

8:00 Introductory Remarks

8:05 Paper 472a: pINDUCER Analysis for the Design of a Nucleation Subsystem for Continuous Slug-Flow Crystallization — ***Mo Jiang***, *Chen Gu, Richard D. Braatz*

8:25 Paper 472b: Understanding Metastable Zone Width Without Nucleation Rate
— ***Venkateswarlu Bhamidi***, *Paul J. A. Kenis, Charles F. Zukoski*

8:45 Paper 472c: Molecular Interactions Between Nanocellulose and Crystallizing Pharmaceuticals
— *Manali Banerjee,* ***Blair Kathryn Brettmann***

9:05 Paper 472d: A New Model for Solubility Prediction to Guide Solvent Selection for Process Development
— ***Michael Lovette***

9:25 Paper 472e: Heterogeneous Nucleation of Small-Molecule Crystals in the Presence of Nanoparticles
— ***Lucrèce Nicoud***, *Leia Dwyer, Allan S. Myerson*

9:45 Paper 472f: The Influence of Solution Conditions on the Self-Assembly of Pre-Nucleation Clusters
— ***Efftychios Hadjittofis***, *Mark A. Isbell, Geoff G. Z. Zhang, Jerry Heng*

10:05 Paper 472g: Simulations and Experiments Validation on the Membrane-Based Response Technology for Nucleation Detection and Crystallization Control
— ***Xiaobin Jiang***, *Wu Xiao, Dapeng Lu, Rui Zhao, Gaohong He*

10:25 Concluding Remarks

(473) Department Heads Forum (Invited Talks)

Wednesday, Nov 1, 8:00 AM
MCC, 205C

Valerie L. Young, Co-Chair
Edward J. Maginn, Co-Chair

Sponsored by:
Department Heads Forum

8:00 Welcoming Remarks

8:03 CAChE Update — ***Mike Henson***

8:23 ABET Accreditation News
— ***Randy Lewis***

8:43 SAChE Resources for Safety
— ***Dan Crowl***

9:03 AIChE Support for Dept. Chairs / Heads — ***David Eckhardt***

9:23 Council for Chemical Research Update — ***Jeff Riemer***

9:38 Salary Survey — ***Geoff Price***

9:58 Panel Discussion: Department Chair to Dean

10:28 Concluding Remarks

(474) Distillation Sequencing and Optimization

Wednesday, Nov 1, 8:00 AM
MCC, M100G

Daniel R. Summers, Chair
Clint P. Aichele, Co-Chair

Sponsored by:
Distillation and Absorption

8:00 Paper 474a: Global Minimization of Multicomponent Distillation Configurations' Total Cost
— ***Parham Mobed***, *Zheyu Jiang, Tony Joseph Mathew, Mohit Tawarmalani, Rakesh Agrawal*

8:25 Paper 474b: A New Minimum-Reflux Calculation Method for Multiple-Feed Distillation Columns Distilling Ideal Multicomponent Mixtures
— ***Zheyu Jiang***, *Mohit Tawarmalani, Rakesh Agrawal*

8:50 Paper 474c: An Easy-to-Use Rule Synthesizes Numerous New Dividing-Wall Columns for Thermally Coupled Distillations
— ***Gautham Madenoor Ramapriya***, *Rakesh Agrawal*

9:15 Paper 474d: Novel Solvent Exchange Distillation System: A Comparison Study with Batch Separations — ***Farhad Fazlollahi***, *Phillip C. Wankat*

9:40 Paper 474e: Experimental and CFD Analysis of a Sieve Tray
— ***Nadine Z. Rafagnim***, *Vitoria A. Castamann, Jaci C. S. C. Bastos, Dirceu Noriler, Henry F. Meier,* ***Marcela Kotsuka Silva***

10:05 Paper 474f: Optimal Design of Advanced Distillation Schemes for Enhancing Energy Efficiency of Close-Boiling Ethylbenzene/Styrene Separation in Plastics Industry
— *Siyao Liu,* ***Chengtian Cui,*** *Jinsheng Sun*

(475) Division Plenary: Materials Engineering & Sciences Division (Invited Talks)

Wednesday, Nov 1, 8:00 AM
MCC, 211B

John G. Ekerdt, Chair
Julie C. Liu, Co-Chair

Sponsored by:
Materials Engineering and Sciences Division

8:00 MESD Poster Award Introductions & Braskem Award Introduction

8:10 Paper 475a: Molecular Understanding, Design and Development of Ultra-Low-Fouling Zwitterionic Materials — ***Shaoyi Jiang***

8:40 Owens-Corning Award Introduction

8:45 Paper 475b: A Scalable Approach to Produce a Diversity of Structured Polymer Colloids
— ***Rodney D. Priestley***

9:15 Paper 475c: Layered Morphologies in Precise Acid-Containing Polyethylenes: Hierarchical Structures and the Implications on Properties — ***Karen I. Winey***

9:40 Paper 475d: Examination of Thin-Film Growth Using Supersonic Molecular Beams and In-Situ Real-Time X-Ray Synchrotron Radiation: From Organic Small-Molecule Semiconductors to Transition Metal Dichalcogenides
— ***James R. Engstrom***

10:05 Paper 475e: Polymer Electrolytes for Electrochemical Energy Devices — ***Yushan Yan***

10:30 Concluding Remarks

(476) Drug Delivery I

Wednesday, Nov 1, 8:00 AM
MCC, 208B

Greg Thurber, Chair
Millicent Sullivan, Co-Chair

Sponsored by:
Engineering Fundamentals in Life Science

8:00 Paper 476a: Immunomodulatory Peptide Amphiphile Micelles for Prophylactic Vaccination — ***Rui Zhang***, *Jake Kramer, Logan Morton, Josiah Smith, Brittany Allen, Caitlin Leeper, Xiaolei Li, Fabio Gallazzi, Tommi White, Bret Ulery*

8:18 Paper 476b: Aptamer-Peptide-Drug Conjugates: Delivery of Precise Synergistic Drug Ratios for Enhanced Cancer Selectivity — ***Anusha Pusuluri***, *Stefano Menegatti, H. Tom Soh, Samir Mitragotri*

8:36 Paper 476c: Heterotrifunctional Scaffolds for Measuring Intracellular Bond Cleavage Kinetics
— ***Michelle Sorkin***, *Christopher A. Alabi*

8:54 Paper 476d: Evaluation of Enzyme-Loaded Nano-Polymersome Treatment on Neurodegenerative Disease — ***Jessica Kelly***, *Doug Martin, Mark E. Byrne*

9:12 Paper 476e: Enhanced Fibrinolysis Using Magnetically Powered Colloidal Microwheels
— ***Dante Disharoon***, *Keith B. Neeves, Tonguc Onur Tasci, David W. M. Marr, Kuldeepsinh Rana*

9:30 Paper 476f: Intracellular and Extracellular Delivery of Proteins and Small Biomolecules via Near-Infrared Light — ***JeongEun Shin***, *Joseph A. Zasadzinski*

9:48 Paper 476g: Repurposing Mechanosensitive Channels to Study Confined 3D Cell Migration
— ***Allen P. Liu***

(477) Environmental Advances in Nuclear and Hazardous Waste Treatment I

Wednesday, Nov 1, 8:00 AM
MCC, 102E

Robert W. Peters, Chair
Thong Hang, Co-Chair
Ramesh Chawla, Co-Chair
Eunsung Kan, Co-Chair

Sponsored by:
Solid and Hazardous Waste

8:00 Paper 477a: Impact of Impurities and Degradation Products During Chemical Processing of High-Level Waste in the Defense Waste Processing Facility — ***Dan P. Lambert***, *J. R. Zamecnik, Wesley H. Woodham, J. David Newell, Matthew S. Williams*

8:30 Paper 477b: Assessment of Dead-End Filtration as Screening Tool for Crossflow Filtration of Hanford Tank Wastes — ***John Geeting***

9:00 Paper 477c: Investigation of High-Level Waste Glass Melting Using X-Ray Computed Tomography
— ***Alexander S. Choi***

9:30 Paper 477d: Chemical Reaction Networks in High-Level Waste (HLW) Treatment at the Defense Waste Processing Facility (DWPF)
— ***Wesley Woodham***, *J. R. Zamecnik*

(478) Environmental Applications of Nanotechnology and Nanomaterials I

Wednesday, Nov 1, 8:00 AM
MCC, 210A/B

Larry Erickson, Chair
Placidus B. Amama, Co-Chair
Tapas K. Das, Co-Chair

Sponsored by:
Environmental Aspects, Applications, and Implications of Nanomaterials and Nanotechnology

8:00 Paper 478a: Nanocarbon-TiO_2 Composites for Photocatalytic Oxidation of Volatile Organic Compounds
— ***Brian Everhart***, *Montgomery Baker-Fales, Eric Banning, Haider Almkhelfe, Huan Wang, Placidus B. Amama*

8:25 Paper 478b: Nanobiosensing Chemicals That Target Nuclear Hormone Receptors: A Rapid, Versatile Cell-Free Protein Synthesis Approach
— ***Bradley C. Bundy***, *Amin Salehi, Miriam Shakalli Tang, Seung Ook Yang, Mark T. Smith, Jeremy Hunt, David W. Wood*

8:50 Paper 478c: Detection of Biocides in Industrial Wastewater Using Pullulan-Encapsulated Microorganisms
— ***Patrick Morkus***, *Damien Parrello, Matthew Csordas, James Rose, Kenneth Byungjun Choi, Carlos D. M. Filipe, David R. Latulippe*

9:15 Paper 478d: Silica Nanoparticle Surface Characteristics Dictate In-Vitro Cytotoxic Behavior
— ***Alexander L. Kelly***, *Kyle D. Paul, Robert D. Arnold, Allan E. David*

9:40 Paper 478e: Development of Novel Nanocatalysts for Environmental Applications Using Helium Isolation Method — ***Alexander Orlov***, *Michael Lindsay, Qiyuan Wu, Shen Zhao, Jiajie Cen, Claron Ridge, Dong Su, Eric A. Stach*

10:05 Paper 478f: Multifunctional Graphene Oxide as Remediation Agent
— ***James G. Radich***, *Rohit Kanungo, Sahm Deravi*

(479) Extractive Separations Fundamentals and Design

Wednesday, Nov 1, 8:00 AM
MCC, M100D

Matthaeus Siebenhofer, Chair
George S. Goff, Co-Chair
Megan E. Donaldson, Co-Chair

Sponsored by: Extractions

8:00 Paper 479a: Effect of Ions on Coalescence in Liquid Two-Phase Systems — ***Jörn Villwock***, *Felix Gebauer, Hans-Jörg Bart, Matthias Kraume*

8:25 Paper 479b: Turbidity Control
— ***Robert Macher-Ambrosch***, *Matthaeus Siebenhofer*

8:50 Paper 479c: Scale-Up Rules for Taylor-Couette Disc Contactor Design
— ***Annika Grafschafter***, *Matthaeus Siebenhofer*

9:15 Paper 479d: Modeling Internal Recycle Within a Mixer-Settler to Aid Extraction Performance
— ***Dave DeSimone***, *Robert Counce, Jack Watson*

9:40 Paper 479e: Liquid-Membrane Separation Process for the Removal of As (III) & As (V) from Drinking Water
— *Soumi Sarkar,* ***Prabirkumar Saha***

10:05 Paper 479f: Extraction of Dyes Using an Aqueous Two-Phase System in Stratified and Slug Flow Regimes of a Microchannel — ***Garima .,*** *S. Pushpavanam*

(480) Fluidization and Fluid-Particle Systems for Energy and Environmental Applications II

Wednesday, Nov 1, 8:00 AM
MCC, 200I

Ali Akhavan, Chair
Luke M. Neal, Co-Chair

Sponsored by:
Fluidization and Fluid-Particle Systems

8:00 Paper 480a: Controlled Removal of Si-Rich Passivation Layer Using a Binary-Solid Fluidized-Bed Reactor for Enhanced Carbon Capture and Storage via Mineralization — *Guanhe Rim, Chengchuan Zhou, Xiaozhou Zhou,* ***Ah-Hyung Alissa Park***

8:18 Paper 480b: Copper Oxide-Based Oxygen Carrier for Chemical-Looping Combustion of Methane: Investigation of Attrition Behaviors and Particulate Formation — *Feng He, Bill Linak,* ***Fanxing Li***

8:35 Paper 480c: Chemical-Looping Gasification (CLG) of Biomass Using a Novel Bimetallic [Copper-Ferrite] Oxygen Carrier — ***Beatrice Muriungi***, *Abolhasan Hashemisohi, Lijun Wang, Abloghasem Shahbazi*

8:52 Paper 480d: Two- and Three-Dimensional Simulation of CO_2 Capture in Fluidized Bed Using Amine-Based Solid Sorbents
— ***Farnaz Esmaeili Rad***, *Hamid Arastoopour, Javad Abbasian*

9:09 Paper 480e: Transition Between Turbulence Regimes in Particle-Laden Channel Flows — ***Jesse Capecelatro***, *Olivier Desjardins, Rodney O. Fox*

9:26 Paper 480f: Experimental Study of a Riser-Based Carbon Stripper in a Solid-Fuel Chemical-Looping-Combustion System — ***Hongming Sun***, *Ningsheng Cai, Mao Cheng, Zhenshan Li*

9:43 Break

10:00 Paper 480h: Investigation of Mixing and Segregation Behavior of Binary Mixture in Liquid-Solid Conical Fluidized Bed Using Radioactive Particle Tracking — ***Lipika Kalo***, *Rajesh Kumar Upadhyay*

(481) Forum Plenary: Sustainable Engineering Forum (Invited Talks)

Wednesday, Nov 1, 8:00 AM
MCC, 101B

Raymond L. Smith, Chair
Ignasi Palou-Rivera, Co-Chair

Sponsored by:
Sustainable Engineering Forum

8:00 Paper 481a: Science with Purpose — ***Maureen Tholen***

8:30 Paper 481b: Some Thoughts on Sustainability: Food, Energy, and Water
— ***Heriberto Cabezas***

9:00 Paper 481c: Industrial Sustainability Enhancement: A Control Perspective — ***Yinlun Huang***

9:30 Paper 481d: Multiscale Life-Cycle Optimization for Sustainable Engineering — ***Fengqi You***

(482) Fundamentals of Electrode Processes I

Wednesday, Nov 1, 8:00 AM
MCC, M100C

Gang Wu, Chair
Hong Yang, Co-Chair
William E. Mustain, Co-Chair

Sponsored by:
Electrochemical Fundamentals

8:00 Paper 482a: Highly Stable Mn-Based Nanocarbon: A New Class of Bifunctional Electrocatalyst for Oxygen Reduction and Evolution Reactions
— *Shiva Gupta,* ***Gang Wu***

8:20 Paper 482b: Density Functional Theory Study of the Oxygen Reduction Reaction in a Graphene Surface Modified with S or N
— ***Elizabeth Montiel-Macias***, *Ysmael Verde-Gómez, Perla B. Balbuena*

8:40 Paper 482c: Highly Stable Nanocarbon Supports for Pt Cathode Catalysts in Polymer Electrolyte Fuel Cells — *Mengjie Chen,* ***Gang Wu***

9:00 Paper 482d: Approaching 2 W·cm^{-2} AEMFCs Through Electrode Engineering and Controlling the Cell Water Content and Balance
— *Travis J. Omasta, Xiong Peng,* ***William E. Mustain***

9:20 Break

9:30 Paper 482e: Design and Engineering of Membraneless Electrolysis Devices
— ***Jonathan Davis***, *Justin Bui, Daniel V. Esposito*

9:50 Paper 482f: Neutron Imaging to Visualize Ion Transport in Electrochemical Cells
— *Yong-ha Kim, Kexin Tang, Ketki Sharma, Sotira Yiacoumi, Hassina Bilheux, Louis Santodonato, Jorge Gabitto,* ***Costas Tsouris***

10:10 Paper 482g: Design of a Novel Electrochemical Membrane Reactor for Hydrogen Production via the S-NH_3 Cycle — ***Raúl Márquez-Montes***, *Raúl Orozco-Mena, Virginia Collins-Martínez, Eduardo Herrera-Peraza, David Chávez-Flores, Víctor Ramos-Sánchez*

(483) Fundamentals of Surface Reactivity

Wednesday, Nov 1, 8:00 AM
MCC, L100F

Eric Walker, Chair
Luke T. Roling, Co-Chair
Samir H. Mushrif, Co-Chair
David W. Flaherty, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

8:00 Paper 483a: Are Undercoordinated Sites Poisoned? A Kinetic Monte Carlo Study of NO Direct Decomposition on Pt55
— ***Benjamin Wei Jie Chen***, *Guowen Peng, Manos Mavrikakis*

8:21 Paper 483b: The Contribution of Nickel and Oxygen Vacancies and of Low-Valent Dopants in Altering the Surface Reactivity of NiO
— ***Jithin John Varghese***, *Samir H. Mushrif*

8:42 Paper 483d: Design of Heterogeneous Catalyst by Stoichiometric Tuning of Intermetallic Gamma-Brass Crystal Structure
— ***Haoran He***, *Anish Dasgupta, Gaurav Kumar, Robert Rioux, Michael J. Janik*

9:03 Paper 483e: Surface Studies of Functional Alcohol Decomposition on Pt and Pd — ***Lesli Mark***, *Hendrik Heinz, Will Medlin*

9:24 Paper 483f: Spectroscopic Insight into the Reactivity of Oxide Electrocatalysts with Water
— ***Kelsey A. Stoerzinger***, *Ryan Comes, Steven R. Spurgeon, Suntharampillai Thevuthasan, Yingge Du, Scott A. Chambers*

9:45 Paper 483g: Understanding and Tuning the Activation of Unsaturated C-C Bonds over Nickel-Based Intermetallic Compounds
— ***Siris Laursen***, *Yang He, Yuanjun Song*

10:06 Paper 483h: Use of Competitive Adsorption with 2,5-Dimethylfuran for the Inhibition of Isomerization and Dimerization Products
— ***Katherine P. Vinter***, *Paul J. Dauenhauer*

(484) Future Automotive Catalysis

Wednesday, Nov 1, 8:00 AM
MCC, L100D

Eleni A. Kyriakidou, Chair
Yang Zheng, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

8:00 Paper 484a: NO Uptake and Desorption on Fe-Modified Pd/ZSM-5: Impact of Pd and Fe Loading
— *Kyle Karinshak,* ***Michael P. Harold***, *Kiran Premchand*

8:18 Paper 484b: Insights into Influencing Factors on Oxygen Storage Characteristics for Ceria-Zirconia Catalysts — ***Jason Wu***, *Giovanni Cavataio*

8:36 Paper 484c: Syntheses of Pd-Doped $CaCo_xZr_{1-}XO_{3-}\delta$ Novel Perovskite-Type Redox Materials for Automotive Emissions Control
— ***Qinghe Zheng***, *Marty Lail*

8:54 Paper 484d: Probing the Oxidation and Reduction Halves of the Cu Redox Cycle During Standard NH_3-Selective Catalytic Reduction of NO_x on Cu-SSZ-13
— ***Ishant Khurana***, *Christopher Paolucci, Atish A. Parekh, Arthur J. Shih, Jonatan D. Albarracin Caballero, Aleksey Yezerets, W. Nicholas Delgass, Jeffrey T. Miller, William Schneider, Rajamani Gounder, Fabio H. Ribeiro*

9:12 Paper 484e: Sulfur Oxidation Studies with Bimetallic Pd/Pt Catalysts
— ***Monique Shauntá Wilburn***, *William Epling*

9:30 Paper 484f: Nature of SO_2-Poisoned Cu-SSZ-13 Catalysts Under Ammonia-Selective Catalytic Reduction (NH_3-SCR) Conditions — ***Arthur J. Shih***, *Hui Li, Ashok Kumar, Juan M. Gonzalez, Ishant Khurana, Christopher Paolucci, Jonatan D. Albarracin Caballero, Atish A. Parekh, Aida Luz Villa, W. Nicholas Delgass, Rajamani Gounder, Aleksey Yezerets, William F. Schneider, Jeffrey T. Miller, Fabio H. Ribeiro*

9:48 Paper 484g: Measurement of the Oxygen Storage Capacity and Its Role in the Catalytic Oxidation — ***Ping Li***, *Chang Yup Seo, Xiaoyin Chen, Yongdan Li, Johannes W. Schwank*

10:06 Paper 484h: Activation of Pd/SSZ-13 in Low-Temperature NO Adsorption for Cold Start Application
— ***Youngseok Ryou***, *JaeHa Lee, Hyokyoung Lee, Changhwan Kim, Do Heui Kim*

(485) Graphene and Carbon Nanotubes: Absorption, Separations, and Transport Processes

Wednesday, Nov 1, 8:00 AM
MCC, 213A/B

Jeffrey A. Fagan, Chair
Shaghayegh Agah, Co-Chair
Geyou Ao, Co-Chair

Sponsored by: Carbon Nanomaterials

8:00 Paper 485a: Ion Transport Through Carbon Nanotubes: A Molecular Dynamics Study
— ***Michelle Aranha***, *Brian J. Edwards*

8:20 Paper 485b: Leveraging Ion Confinement in Porous Carbon Nanomaterials for Rapid Energy Storage — ***Alexander J. Pak***, *Gyeong S. Hwang*

8:40 Paper 485c: Water Wettability of Graphitic Surface: Contaminants, Defect and Roughness — ***Lei Li***

9:00 Paper 485d: Brownian Diffusion of Single-Walled Carbon Nanotubes in Rock-Like Colloidal Crystal Pores
— ***Zhao Tang,*** *Shannon L. Eichmann, Robert Headrick, F. C. MacKintosh, Matteo Pasquali*

9:20 Paper 485e: Developments in the Modulation of Carbon Nanotube Photoluminescence — ***Daniel Heller***, *Daniel Roxbury, Januka Budhathoki-Uprety, Prakrit Jena, Thomas Galassi, Ryan Williams, Rachel Langenbacher, Rune Frederiksen, Christopher Horoszko*

9:40 Paper 485f: Thermal Transport and Electronic Properties of Pure and Hydrogenated Electron-Irradiated Graphene — ***Asanka Weerasinghe***, *Ashwin Ramasubramaniam, Dimitrios Maroudas*

10:00 Paper 485g: Modelling the Effect of Electron Beam Irradiation on the Thermal Conductivity of Monolayer Graphene — ***Srilok Srinivasan***, *Ganesh Balasubramanian*

(486) Honoring the Lifelong Achievements of Dr. Jerry Johanson

Wednesday, Nov 1, 8:00 AM
MCC, 200J

Kerry Johanson, Chair
Shrikant Dhodapkar, Co-Chair

Sponsored by:
Solids Flow, Handling and Processing

8:00 Paper 486a: Evolution of Powder Testers – Key Challenges and Opportunities — ***Tim Freeman***

8:20 Paper 486b: Predicting Segregation in Flowing Granular Materials — ***Richard M. Lueptow***

8:40 Paper 486c: Making Solids Flow in Hoppers Using Passive Activation and Diamondback Hoppers
— ***Lee Dudley***

9:00 Paper 486d: The Impact and Use of Diamondback Hoppers in the Paper, Pulp and Biomass Industries
— ***Bertil Stromberg***

9:20 Paper 486e: A Historical Perspective: The Impact of the Development of Bulk Solids Handling in Australia — ***Alan Roberts***

9:40 Paper 486f: Functionalization of Powders by Modifications of Powder Size and Morphology
— ***Joerg Theuerkauf***

10:00 Paper 486g: Bulk Solids Flow Theory, Then and Now: Pointing a Direction Towards the Future
— ***Jerry R. Johanson***

(487) Important Issues in Professional Development, Including the Management Division's Award Recipient Presentation (Invited Talks)

Wednesday, Nov 1, 8:00 AM
MCC, L100G

Caroline Reynolds, Chair
Joseph Cramer, Co-Chair

Sponsored by:
Professional Development

8:00 Paper 487a: Group-Contribution Coarse-Grained Molecular Simulations of Polystyrene Melts and Polystyrene Solutions in Alkanes Using the SAFT-γ Force Field — ***Robert Zeller***

9:00 Paper 487b: Critical Issues in Environmental Cleanup of Former Nuclear Sites — ***Kenneth Rueter***

9:45 Paper 487c: Your Career Path Is like a Distillation Column
— ***Tianxing Cai***

10:15 Q&A — All Speakers and Audience

(488) Interfacial Transport Phenomena

Wednesday, Nov 1, 8:00 AM
MCC, M100A

Mark Kastantin, Chair
Stephen M. Martin, Co-Chair
Sergey Vasenkov, Co-Chair

Sponsored by: Interfacial Phenomena

8:00 Welcoming Remarks

8:03 Paper 488a: Portable Smartphone-Enabled Capillary-Based Viscometer and Tensiometer
— ***Jose C. Contreras-Naranjo***, *Xiaorui Dong, Victor M. Ugaz*

8:19 Paper 488b: An Experimental Study of a Liquid Drop Impinging on a Liquid Pool — ***Manas Ranjan Behera***, *Anirvan Dasgupta, Sudipto Chakraborty*

8:35 Paper 488c: Arresting Dissolution by Interfacial Rheology Design
— ***Peter J. Beltramo***, *Manish Gupta, Alexandra Alicke, Jan Vermant*

8:51 Paper 488d: The Importance of the Amorphous Material Interface in the Measurement of Thermodynamic Parameters, Using Inverse Gas Chromatography
— ***Eftychios Hadjittofis***, *Geoff G. Z. Zhang, Jerry Heng*

9:07 Paper 488e: Mechanisms of Dynamic Wetting Failure in the Presence of Soluble Surfactants
— ***Chen-Yu Liu***, *Marcio S. Carvalho, Satish Kumar*

9:23 Paper 488f: Electrostatic Assist of Liquid Transfer in Printing Processes — ***Chung-Hsuan Huang***, *Satish Kumar*

9:39 Paper 488g: Analysis of Temperature Gradient Zone Melting and Annealing for Mitigation of Second-Phase Particles in Single Crystals
— ***Kerry Wang***, *Nathan T. Morgan, Jeffrey J. Derby*

9:55 Paper 488h: In-Situ Partitioning Measurements of Multiple Fermentation End-Products into Lipid Membranes — ***Geoffrey D. Bothun***, *John Nunes, Carmen Scholz, Javier Sanchez*

10:11 Paper 488i: Synchronization and Traveling Waves Within Arrays of Electrostatic Oscillators
— ***Shashank Pandey***, *Yong Dou, Charles A. Cartier, Mikolaj Kowalik, Kyle J. M. Bishop*

10:27 Concluding Remarks

(489) Ionic Liquids: Thermodynamics and Properties

Wednesday, Nov 1, 8:00 AM
MCC, 103B

Zhang Suojiang, Chair
Yizu Zhu, Co-Chair
Xiangping Zhang, Co-Chair

Sponsored by:
Innovations of Green Process Engineering for Sustainable Energy and Environment

8:00 Paper 489a: Thermally Robust Molten Salts & Ionic Liquids: Thermodynamics Properties and Phase Behavior — ***Kevin N. West***, *Benjamin Siu, Alexander Badini, Mohammad Soltani, Cody G. Cassity, Richard A. O'Brien, James H. Davis Jr.*

8:17 Paper 489b: Structure and Application of Hydrogen Bond in Ionic Liquid — ***Kun Dong Sr.***

8:34 Paper 489c: A Molecular Understanding of Cellulose Dissolution in Aqueous Ionic Liquids
— ***Brooks D. Rabideau***

8:51 Paper 489d: Freezing Point Determination of Water–Ionic Liquid Mixtures — ***Suojiang Zhang***, *Anne S. Meyer*

9:08 Paper 489e: Effects of the Dielectric Contrast and Hydrogen Bond Between Polymer and Ionic Liquid on the Shift in the Critical Point of the Spinodal from a Polymer-Poor to a Polymer-Rich Region
— ***Issei Nakamura***

9:25 Paper 489f: Assessing the Reliability of Computing Ion Pair Lifetimes and Diffusivity to Predict Experimental Viscosity Trends of Ionic Liquids — ***Michael T. Humbert***, *Yong Zhang, Edward J. Maginn*

9:42 Paper 489g: Ammonia Absorption in Ionic Liquids — ***Tugba Turnaoglu***, *Mark B. Shiflett*

9:59 Paper 489h: Solubilities and Diffusivities of Oxygen in Ionic Liquids for Electrochemical Applications
— ***Tangqiumei Maggie Song***, *Oscar Morales, Kan Huang, Hongfei Jia, Joan F. Brennecke*

10:16 Paper 489i: The Formation and Regulation Mechanism of Meso-Structure of Ionic Liquids
— ***Suojiang Zhang***

(490) Lignocellulosic Materials

Wednesday, Nov 1, 8:00 AM
MCC, 200B

Amar K. Mohanty, Chair
Manju Misra, Co-Chair

Sponsored by:
Forest and Plant Bioproducts Division

8:00 Paper 490a: Continuous Distillation of Fast-Pyrolysis Bio-Oils
— ***Yaseen Elkasabi***

8:25 Paper 490b: Lignin Fillers in Polylactic Acid Composite: The Effects of Impurities in Lignin and Lignin Type — ***Xianglan Bai***, *Yiwei Gao, Wangda Qu*

8:50 Paper 490c: Effect of Polyethylene Terephthalate in Producing Carbon Fiber from Pyrolytic Lignin — ***Wangda Qu***, *Xianglan Bai*

9:15 Paper 490d: Sustainable Graphenic Fixed-Bed Hybrid Adsorbents: Green Synthesis and Application
— *Sreenivasan Sreeprasad, Caroline Louis, Davis Hendricks, Joseph Lawrence,* ***Srikanth Pilla***

9:40 Paper 490e: Large-Scale Implementation of a New Technique for Sugar Extraction and Conversion to Furans from Biomass Hydrolysates
— ***Jeremy Schreur***, *Sasidhar Varanasi, Patricia Relue*

10:05 Paper 490f: Microwave-Assisted Depolymerization of Lignin to Phenolics in Polar Solvents — ***Piyali Dhar, R. Vinu***

(491) Metabolic and Process Engineering for Value-Added Products from Food Processing

Wednesday, Nov 1, 8:00 AM
MCC, 206A/B

Shang-Tian Yang, Chair
Fangfang Liu, Co-Chair
Le Yu, Co-Chair

Sponsored by: Food

8:00 Paper 491a: Quality Improvement of PhilRice "Tapuy" by Ultrafiltration Hollow Fiber Membrane
— ***Michelle C. Almendrala***, *Evelyn H. Bandonill, Marissa V. Romero*

8:18 Paper 491b: Novel Applications of Walnut Husk Extracts
— ***Jonathan E. Wenzel***, *Scott Constine, Erin Kissick, Elijah Ward, Lihua Wang, Michelle Ammerman, Cheryl Samaniego*

8:36 Paper 491c: Nutritional Value Improvement of Corn Ethanol Co-Product by Yeast Engineering
— ***Yanmei Zhang,*** *Jingyu Wang, Bo Hu*

8:54 Paper 491d: Effects of Artificial Electron Carriers on Increasing NADH Availability, Acetate Re-Assimilation and Butyric Acid Production by *Clostridium tyrobutyricum*
— ***Hongxin Fu***, *Jufang Wang, Shang-Tian Yang*

9:12 Paper 491e: Zinc-Mediated Pleiotropic Effects and Regulatory Mechanism on Acetone-Butanol-Ethanol (ABE) Fermentation by *Clostridium acetobutylicum*
— ***Wu Youduo,*** *Chuang Xue, Lijie Chen*

9:30 Paper 491f: A Computational Modeling to Integrate Multi-Omics in *Clostridium cellulovorans* to Guide Metabolic Engineering — ***Jianfa Ou***, *Ningning Xu, Chao Ma, Patrick Ernst, X. Margaret Liu*

9:48 Paper 491g: (Keynote) Increasing Tolerance to High Salt Concentrations in Acid Hydrolysate of Cassava Pulp by Cell Immobilization in a Static-Bed Fermentor — ***Nuttha Thongchul***, *Siriporn Ounaeb, Varunee Pimtong, Sitanan Thitiprasert*

(492) Microbial Engineering for Human Health

Wednesday, Nov 1, 8:00 AM
MCC, 205A/B

Nikhil U. Nair, Chair

Sponsored by:
Microbiomes and Microbial Communities

8:00 Paper 492a: Probiotic Escherichia coli Inhibits Biofilm Formation of Pathogens — ***Kuili Fang***, *Seok Hoon Hong*

8:25 Paper 492b: Understanding and Engineering the Metabolic Environment of a Healthy Skin Microbiome
— ***Collin M. Timm***, *Kristin Loomis, Bryan Brensinger, Jared Evans, David Karig*

8:50 Paper 492c: Micro-Droplet Co-Cultivation and Characterization of Vaginal Bacteria — ***Corine Jackman***, *Xiaoxia (Nina) Lin*

9:15 Paper 492d: Targeted Species Removal in a Model Microbiome via Phage Lytic Enzymes
— *Amala Bhagwat, Jonathan S. Dordick,* ***Cynthia H. Collins***

9:40 Paper 492e: Programming Beneficial *E. coli* to Sense and Kill *Vibrio cholerae*, the Causative Agent of Cholera
— ***Chueh Loo Poh***, *Maciej B. Holowko, Premkumar Jayaraman*

(493) Mixing Scale-Up/Scale-Down Issues in Pharmaceutical and Biopharmaceuticals Processes

Wednesday, Nov 1, 8:00 AM
MCC, 102D

Piero Armenante, Chair
Luis Sierra, Co-Chair

Sponsored by:
North American Mixing Forum

8:00 Paper 493a: Numerical Study on Mixing and Crystallization in an Impinging Jet Mixer — ***Jingcai Cheng***, *Chao Yang, Zai-Sha Mao, Minghui Xie*

8:22 Paper 493b: Power Dissipation in Pharmaceutical Reactors and Vessels Equipped with a Retreat-Blade Impeller
— *Chadakarn Sirasitthichoke,* ***Piero M. Armenante***

8:44 Paper 493c: Proven Results of Converting Batch Mixing Systems to Flexible Continuous Inline Blending System — ***John R. Schott***

9:06 Paper 493d: The Effect of Particle Shape in Drum Mixers
— ***Nicolin Govender***, *Daniel Wilke, Sarah Fathollahi, Raj Rajamani, Johannes G. Khinast*

TECHNICAL SESSIONS 2017

(494) Multiphase Flow Characterization
Wednesday, Nov 1, 8:00 AM
Hilton, Conrad D

Ali Mohraz, Chair
Lilian Hsiao, Co-Chair

Sponsored by: Fluid Mechanics

8:00 Paper 494a: Probing Viscosity of Complex Emulsions with Micro-Rheometry — *Archit Dani, Shweta Narayan,* ***Cari S. Dutcher***

8:15 Paper 494b: The Study on Mechanism of Flow Distribution and Its Optimization in a Spray Column — ***Penghui Wang****, Gance Dai*

8:30 Paper 494c: Design of Optimal Elastomeric Valves to Achieve Spatiotemporal Control of Droplets in Microfluidic Networks — ***Sarojini Tiwari****, Jeevan Maddala*

8:45 Paper 494d: Analysis of Interfacial Forces of a Slurry Bubble Column — *Bruna L. Mees, Tatiana Matiazzo, Jaci C. S. C. Bastos, Henry F. Meier,* ***Marcela Kotsuka Silva***

9:00 Paper 494e: Semi-Batch Liquid-Liquid Taylor Vortex Flow: Comparison of 3-D and 2-D Eulerian-Eulerian CFD Simulations and Experimental Measurements for Fluid Flow Patterns and Droplet Holdup — *John Lavey, Arya Haghighat, Charlton Campbell, Xi Gao,* ***Bo Kong****, Meesha Legg, Michael Olsen, R. Dennis Vigil*

9:15 Paper 494f: Hydrodynamics of Gas-Liquid Bubbly Flow at High Pressure and Temperature — ***Zhen Tian***

9:30 Paper 494g: Experiments on Bubble Behaviors in Three-Phase Internal-Loop Airlift Reactor Using Optical Fiber Probe Measurements — ***Yongxiang Gao***

9:45 Paper 494h: Flow Properties of Gas Hydrate Slurry in Oil-Dominated Transportation Systems — ***Lin Ding****, Bohui Shi, Yang Liu, Shangfei Song, Jing Gong*

10:00 Paper 494i: Relationship Between Flow Pattern in Cyclone Classifier and Classification Process — ***Zhanpeng Sun****, Guogang Sun, Yan Du*

10:15 Paper 494j: Dynamic Liquid Level Effect on Bubble Properties in Industrial Bubble Column Without Internal by Using Four-Point Optical Fiber Probe Technique — ***Hayder Al-Naseri****, Joshua P. Schlegel, Muthanna H. Aldahhan*

(495) Nanomaterials for Light Harvesting and Novel Photophysical Phenomenon II
Wednesday, Nov 1, 8:00 AM
MCC, 200G

Sang Eon Han, Chair
William A. Tisdale, Co-Chair
Ayaskanta Sahu, Co-Chair

Sponsored by: Nanomaterials for Applications in Energy and Biology

8:00 Paper 495a: Enhanced Optoelectronic Functionality of Photovoltaic 2D Crystal-Nanoantenna Hybrids — ***D. Keith Roper****, Gregory T. Forcherio, Jeremy Dunklin, Mourad Benamara, Luigi Bonacina, Yana Vaynzof, Claudia Backes*

8:20 Paper 495b: High-Efficiency Dynamic Lighting with Transition Metal Elements as Sensitizers — *Pragathi Darapaneni, Raju Kumal, Alexander Meyer, Mohammad Saghayezhian, Louis Haber, Kenneth Lopata, Ward Plummer, Yuanbing Mao,* ***James Dorman***

8:40 Paper 495c: Mechanism and Design Principles for Directing Energy Flow in Multicomponent Plasmonic Systems — ***Steven Chavez****, Umar Aslam, Suljo Linic*

9:00 Paper 495d: Semiconducting Halide Perovskite Nanomaterials and Heterojunctions — ***Letian Dou***

(496) Nanotechnology for Biotechnology and Pharmaceuticals
Wednesday, Nov 1, 8:00 AM
MCC, 212A/B

Richey Davis, Chair
Sutapa Barua, Co-Chair

Sponsored by: Bionanotechnology

8:00 Paper 496a: Tumor-Penetrating Aerosol Nanocomposite Microparticles for the Treatment of Lung Cancer — ***Elisa A. Torrico-Guzmán****, Samantha A. Meenach*

8:15 Paper 496b: Monitoring Nanoparticle Stability and Mobility in Whole Blood and Tissues In Situ — *Ana C. Bohorquez, Mythreyi Unni, Andreina Chiu-Lam, Sayali Belsare, Lori Rice, Chris Pampo, Dietmar Siemann,* ***Carlos Rinaldi***

8:30 Paper 496c: On-Chip Manufacturing of Synthetic Proteins for Point-of-Care Therapeutics — ***Jiayuan Sheng****, Travis Murphy, Chang Lu, Xueyang Feng*

8:45 Paper 496d: Formulation of Stable Nanosuspensions of a Novel Malaria Therapeutic Through Polymer-Directed Precipitation — ***Kurt D. Ristroph****, Hoang Lu, Ellen Dobrijevic, Simon A. McManus, Yingyue Zhang, Jie Feng, William D. Mulhearn, Robert Prud'homme*

9:00 Paper 496e: Engineering Surface-Functionalized, Intelligent Hydrogel Nanoparticles with Tunable Release Properties — ***Angela Wagner****, Noor Al-Sayyad, Alexandria Lawrence, Nicholas Peppas*

9:15 Paper 496f: Nanocarrier-Enhanced Photoimmunotherapy for Cancer — ***Huang-Chiao Huang****, Michael Pigula, Yanyan Fang, Tayyaba Hasan*

9:30 Paper 496g: Nanoharvesting of Therapeutics from Living Plant Cultures by Engineered Mesoporous Silica Nanoparticles — ***M. Arif Khan****, Stephen E. Rankin, John M. Littleton, Barbara L. Knutson*

9:45 Paper 496h: Degradation of Phospholipid Vesicles by Phospholipases — ***Pin Zhang****, Veronica Villanueva, Alexander Donovan, Joseph Kalkowski, Chang Liu, Wei Bu, Binhua Lin, Ying Liu*

10:00 Paper 496i: Oral Delivery of siRNA Lipid Nanoparticles: Fate in the GI Tract — ***Rebecca Ball****, Palak Bajaj, Kathryn A. Whitehead*

10:15 Paper 496j: Particle-Engineering Surface-Functionalizable Fluorescently Labeled Polymeric Nanoparticles for Drug Delivery — ***Ami Jo****, Rui Zhang, Judy S. Riffle, Richey M. Davis*

(497) Networked, Decentralized, and Distributed Control
Wednesday, Nov 1, 8:00 AM
MCC, 103D

Joseph Sangil Kwon, Chair
Mona Bavarian, Co-Chair

Sponsored by: Systems and Process Control

8:00 Paper 497a: Distributed Model Predictive Control of Complex Plants: A Systematic Study of Decomposition Effects — ***Davood Babaei Pourkargar****, Ali Almansoori, Prodromos Daoutidis*

8:21 Paper 497b: Dynamic Real-Time Optimization of Distributed MPC Systems Using Rigorous Closed-Loop Prediction — ***Hao Li****, Christopher L. E. Swartz*

8:42 Paper 497c: Graph-Theoretic Approach for the Synthesis of Distributed Control Architecture — ***Sujit S. Jogwar***

9:03 Paper 497d: Event-Based Networked Control of Distributed Process Systems with Sensor-Controller Communication Failures — ***Da Xue****, Nael H. El-Farra*

9:24 Paper 497e: Distributed Safeness Index-Based Predictive Control for Enhanced Process Operational Safety — ***Fahad Albalawi****, Helen Durand, Panagiotis D. Christofides*

9:45 Paper 497f: Two-Point Constraint Control of Water Quality in Distribution Networks — ***Abhilasha Maheshwari***

10:06 Paper 497g: Relative Time–Averaged Gain Array for Distributed Control Architecture Design — ***Wentao Tang****, Davood Babaei Pourkargar, Prodromos Daoutidis*

(498) NH_3 Energy Overview and Safety
Wednesday, Nov 1, 8:00 AM
MCC, 101F/G

Sponsored by:
NH_3 Energy$^+$ — Enabling Optimized, Sustainable Energy and Agriculture

8:00 Paper 498a: NH_3: The Optimal Alternative Fuel — ***Norman K. Olson***

8:18 Paper 498b: Dutch Initiatives to Store Sustainable Energy in the Form of Ammonia — ***Johannes Pieter Vrijenhoef***

8:36 Paper 498c: Nitrogen-Based Fuels: Renewable Hydrogen Carriers — ***Gideon S. Grader****, Michael Epstein, Ayillath K. Deepa, Oren Elishav, Gennady E. Shter, Bar Mosevitzky*

8:54 Paper 498d: Addressing the Critical Tasks Associated with Emergency Response to an Ammonia Incident — ***Gary Smith***

9:12 Paper 498e: Ammonia Fuel Safety — ***Trevor Brown***

9:30 Paper 498f: Ammonia Renewable Energy Fuel Systems at Continental Scale: Transmission, Storage, and Integration for Deep Decarbonization of World's Largest Industry at Lower Cost Than Electricity — ***William C. Leighty***

9:48 Paper 498g: Comprehensive Evaluation of NH_3 Production and Utilization Options for Clean Energy Applications — ***Greg Vezina***

10:06 Paper 498h: The Role of "Green" Ammonia in Decarbonising Energy Systems: Practical Demonstration and Economic Considerations — ***Ian Wilkinson***

(499) Novel Nanoparticles and Nanostructured Materials for Catalysis — Influence of Particle Size
Wednesday, Nov 1, 8:00 AM
MCC, 200H

Steven R. Saunders, Chair
Chao Wang, Co-Chair

Sponsored by: Nanoparticles

8:00 Paper 499a: Colloidal Pd Nanoparticle Synthesis: The Effect of Ligand-Metal-Solvent Thermodynamics on Kinetics and Final Size — ***Wenhui Li****, Christopher Wooten, Sergei A. Ivanov, Saeed Mozaffari, Michael G. Taylor, Giannis Mpourmpakis, Ayman M. Karim*

8:20 Paper 499b: Switchable Surfactants for the Preparation of Monodisperse, Supported Nanoparticle Catalysts — ***Kristin Bryant****, Gasim Ibrahim, Steven R. Saunders*

8:40 Paper 499c: Colloidal Iron Nanoparticles Provide Size Control in the Catalytic CO Hydrogenation Reaction — ***Viacheslav Iablokov****, Anca Meffre, Bruno Chaudret, Norbert Kruse*

9:00 Paper 499d: Selective Dehydrogenation and Oxidation Reactions on NiAu Alloys at the Single-Atom Limit — ***Georgios Giannakakis****, Antonios Trimpalis, Junjun Shan, Maria Flytzani-Stephanopoulos*

9:20 Paper 499e: The Effect of Pd Size on TiO_2 for Photocatalytic NO_x Removal — ***Sotiris E. Pratsinis***

9:40 Paper 499f: Exploring Fundamental Properties of Fe- and Mn-Promoted Rh Catalysts for Syngas Conversion to Higher Alcohols — ***Florian Göltl****, Yifei Liu, Insoo Ro, George W. Huber, James A. Dumesic, Manos Mavrikakis*

10:00 Paper 499g: Controlling Energy Flow in Plasmonic Photocatalysis Through the Design of Hybrid Plasmonic Nanostructures — ***Umar Aslam****, Steven Chavez, Suljo Linic*

(500) Panel: Precompetitive Collaboration
Wednesday, Nov 1, 8:00 AM
MCC, 204A/B

Jean W. Tom, Chair
Joe Hannon, Co-Chair

Sponsored by:
Pharmaceutical Discovery, Development and Manufacturing Forum

8:00 Paper 500a: NIIMBL: The National Institute for Innovation in Manufacturing Biopharmaceuticals — ***Kelvin H. Lee***

8:20 Paper 500b: The TransCelerate Comparator Network: Transforming the Supply Chain for Clinical Comparator Medicines — ***Nishchal Chudasama***

8:40 Paper 500c: Accelerating Pharmaceutical Development Through Precompetitive Collaboration: The Enabling Technologies Consortium — ***Srinivas Tummala****, **Joshua D. Engstrom****, Jean W. Tom, Margaret Faul*

9:00 Paper 500d: CMAC: A Partnership Approach to Precompetitive Collaboration for Pharmaceutical Manufacturing Research — ***Alastair J. Florence***

9:20 Paper 500e: A Perspective on a Pre-Competitive NSF Engineering Research Center Focused on Pharmaceutical Manufacturing: C-SOPS — ***Douglas Hausner***

9:40 Paper 500f: The Development of an Interactive Knowledge Epicenter for the Advancement of Continuous Manufacturing — ***Philip Donnellan****, Lawrence De Belder*

10:00 Panel Discussion

(501) Pathways to Thermal Deconstruction
Wednesday, Nov 1, 8:00 AM
MCC, 101I

Phillip R. Westmoreland, Chair

Sponsored by:
Thermal Deconstruction of Biomass

8:00 Paper 501a: Thermal Deconstruction on Lignocellulosic Biomass — ***Robert C. Brown***

8:25 Paper 501b: Overcoming Challenges of Integrating Pretreatment with Enzymatic Saccharification and Microbial Fermentation Using Ionic Liquids (ILs) or Bionic Liquids (BILs) — ***Blake Simmons****, Feng Xu, Jian Sun, N.V.S.N. Murthy Konda, Jian Shi, Tanmoy Dutta, Corinne D. Scown, Seema Singh*

8:50 Paper 501c: Biomass Deconstruction Towards Total Carbon Utilization for Future Biorefineries — ***Charles M. Cai****, Abhishek Patri, Barmak Mostofian, Bhogeswararao Seemala, Ninad D. Kothari, Thanh Yen Nguyen, Yunqiao Pu, Loukas Petridis, Micholas Smith, Xiaolin Cheng, Jeremy Smith, Arthur J. Ragauskas, Phillip Christopher, Rajeev Kumar, Charles E. Wyman*

9:15 Paper 501d: Lignocellulosic Biomass Fractionation and Upgrading Strategies Using Gamma Valerolactone as Solvent — ***David Martin Alonso****, Sikander H. Hakim, Shengfei Zhou, Wangyun Won, Omid Hosseinaei, Jingming Tao, Valerie Garcia-Negron, Ali Hussain Motagamwala, Max A. Mellmer, Kefeng Huang, Carl J. Houtman, Nicole Labbé, David Harper, Christos Maravelias, Troy Runge, James Dumesic*

9:40 Paper 501e: On the Synergy Between Non-Thermal and Thermal Catalytic Deconstruction of Waste Lignocellulosic Materials — ***Roberto Rinaldi***

10:05 Paper 501f: Stabilization with Aldehydes for the High Yield Production of Targeted Monomer Mixtures from Lignin During Integrated Biomass Depolymerization — ***Jeremy S. Luterbacher***

(502) Pharmaceutical Process Development and Pilot Plants
Wednesday, Nov 1, 8:00 AM
MCC, 102C

Elie Chaaya, Chair

Sponsored by: Pilot Plants

8:00 Paper 502a: Scale-Up Modelling and Analysis of a Pharmaceutical Crystallization Process — ***Merve Öner****, Getachew S. Molla, Michael Frederick Freitag, Stuart Michael Stocks, Jens Abildskov, Gürkan Sin*

8:25 Paper 502b: Removal of Impurity from API and Reduction of Agglomeration During Drying — ***Onkar Manjrekar****, Howard E. Morton, Jie Chen, Lijie Cui, David Barnes, Jose Napolitano, Jeff Hartnell, Jeff Bien, Elie Chaaya, Subramanya Nayak, Shailendra Bordawekar*

8:50 Paper 502c: Developing Scale-Up Approach for Fast Chemical Reactions in Continuous Flow — ***Plamen Grigorov***

9:15 Paper 502d: Viscoelastic Properties and Dissolution Kinetics of Amorphous Drug Dispersion Films, Utilizing the Quartz Crystal Microbalance — ***Mark A. Isbell****, Geoff G. Z. Zhang, J. Y. Y. Heng*

9:40 Paper 502e: Improving the Dissolution of Ibuprofen by Co-Milling of Ibuprofen and MCC Mixture in a Ball Mill — ***Sophia Varghese****, Chinmay Ghoroi*

(503) Process Intensification Through Process Systems Engineering
Wednesday, Nov 1, 8:00 AM
MCC, 101D

Ankur Kumar, Chair
M. M. Faruque Hasan, Co-Chair

Sponsored by:
Systems and Process Design

8:00 Paper 503a: Innovative Design and Systematic Process Intensification Using Building Blocks — ***M. M. Faruque Hasan****, Salih E. Demirel, Jianping Li, Shachit S. Iyer, Akhil Arora*

8:21 Paper 503b: Modeling and Simulation of a Hybrid Adsorptive-Membrane Reactor (HAMR) for Intensification of the Water-Gas Shift (WGS) Reaction Process — ***Secgin Karagoz****, Theo Tstosis, Vasilios Manousiouthakis*

8:42 Paper 503c: Intensification of Chemical Processes via Periodic Operation — *Lingqing Yan, Thomas F. Edgar, Michael Baldea*

9:03 Paper 503d: Intensification of the Hydride Vapor-Phase Epitaxy Manufacturing Process for Solar Devices — ***Min Yao****, James B. Rawlings, Thomas F. Kuech*

9:24 Paper 503e: Process Intensification of Reactive Separator Networks Through the IDEAS Conceptual Framework — ***Flavio da Cruz****, Vasilios Manousiouthakis*

9:45 Paper 503f: Intensified Reaction-Separation Schemes — *Evangelia Koumaditi, John M. Woodley,* ***Rafiqul Gani***

10:06 Paper 503g: Process Intensification of Large-Scale Continuous Biobutanol Production via a Multi-Feed Bioreactor with In-Situ Gas Stripping — ***Jonathan P. Raftery****, M. Nazmul Karim*

(504) Protein Engineering I: Therapeutics
Wednesday, Nov 1, 8:00 AM
MCC, 207A/B

Benjamin J. Hackel, Chair
James Van Deventer, Co-Chair

Sponsored by: Bioengineering

8:00 Paper 504a: Engineering and Profiling the Substrate Specificity of Human Proteases for Therapeutic Applications — ***Carl A. Denard****, Rasha Yaghi, Brent L. Iverson*

8:18 Paper 504b: A Novel Transthyretin Peptide Mimic as a Therapeutic for Alzheimer's Disease — ***Kayla Pate****, Regina M. Murphy*

8:36 Paper 504c: Directing Reversible Cell-Cell Interactions with Evolved Fibronectin Domains
*— **Clifford M. Csizmar**, Lawrence A. Stern, Jacob R. Petersburg, Benjamin J. Hackel, Carston R. Wagner*

8:54 Break

9:12 Paper 504e: Enhancing the Chemical Versatility of Yeast Display to Target the Tumor Microenvironment
*— Jessica T. Stieglitz, Haixing P. Kehoe, Gregory I. Berumen, Hanan Z. Lane, Laura B. Quinto, **James Van Deventer***

9:30 Paper 504f: Tunable Thermal Bioswitches for In-Vivo Control of Biological Therapeutics *— **Dan Piraner**, Mohamad Abedi, Brittany Moser, Audrey Lee-Gosselin, Mikhail G. Shapiro*

9:48 Paper 504g: Now You See Me, Now You Don't: Building Better Biologics Through Immune Evasion *— **Karl E. Griswold***

(505) Protein Structure, Function, and Stability I: Engineering Technology
Wednesday, Nov 1, 8:00 AM
MCC, 208A

Mark A. Blenner, Chair
Derek Englert, Co-Chair

Sponsored by: Bioengineering

8:00 Paper 505a: Engineering Glucose-Responsive Insulin for Self-Regulated Diabetes Therapy
*— **Abel B. Cortinas**, Kevin Daniel, Daniel G. Anderson*

8:18 Paper 505b: Expression of EK Fusion Proteins to Enhance Protein Kinetics and Stability *— **Erik J. Liu**, Shaoyi Jiang*

8:36 Paper 505c: Regulation of Multispanning Membrane Protein Topology via the Post-Translational Flipping of Charged Protein Elements *— **Reid Van Lehn***

8:54 Paper 505d: Characterization of Pro-Regions in Mammalian Growth Factors Using Deep Sequencing and Yeast Surface Display *— **Angélica V. Medina-Cucurella***

9:12 Paper 505e: Intrinsically Disordered Proteins as Sensors of Membrane Curvature *— **Wade F. Zeno**, Jeanne C. Stachowiak*

9:30 Paper 505f: Effect of Secondary Structure of Cell-Penetrating Peptides on Their Interaction with Fungal Cells *— Zifan Gong, **Amy J. Karlsson***

9:48 Paper 505g: Predicting and Engineering Protein Complex Structures, from Antibodies to Glycoproteins *— **Jeffrey Gray***

(506) Reaction Engineering for Biomass Conversion
Wednesday, Nov 1, 8:00 AM
MCC, L100C

Fernando Resende, Chair
M. Toufiq Reza, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

8:00 Paper 506a: Microwave-Responsive CNT/Polyaniline Core/Shell Structured Catalysts for High Energy Efficiency in Saccharide-HMF Conversion *— **Tuo Ji**, Jiahua Zhu*

8:21 Paper 506b: Modeling Residence Time Distribution and Physical Parameters in Horizontal Screw Hydrolysis Reactors
*— **David A. Sievers**, Jonathan J. Stickel*

8:42 Paper 506c: Mo@Pt Overlayer as Effective Catalysts for Hydrodeoxygenation of Guaiacol and Anisole *— **Qinghua Lai**, Chen Zhang, Joseph Holles*

9:03 Paper 506d: Reaction Engineering for Bio-Renewable Furan-Derived Surfactants
*— **Kristeen Esther Joseph**, Dae Sung Park, Christoph Krumm, Michael Tsapatsis, Raul F. Lobo, Dionisios G. Vlachos, Paul J. Dauenhauer*

9:24 Paper 506e: Upgrading of In-Situ Catalytic Fast-Pyrolysis Bio-Oil to Hydrocarbon Fuels *— **Daniel Santosa**, Huamin Wang, Foster Agblevor*

9:45 Paper 506f: Bio-Terephthalic Acid Synthesis from Cross-Metathesis of Unsaturated Carboxylic Acids and Consecutive One-Pot Cycloaddition and Aromatization Reactions
*— **Erisa Saraçi**, Raul F. Lobo*

10:06 Paper 506g: Lignin Hydrogenolysis over Nickel-Based Bimetallic Catalysts
*— **Jiaguang Zhang**, Ning Yan*

(507) Reaction Engineering in Pharmaceuticals and Fine Chemicals
Wednesday, Nov 1, 8:00 AM
MCC, L100B

Gaurav Giri, Chair
Anuj A. Verma, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

8:00 Paper 507a: Continuous-Flow Nitration: Research and Process Development *— **Anuj A. Verma**, Kaid Harper*

8:20 Paper 507b: On-Demand Medicinal Chemistry and Compound Synthesis in Oscillating Droplets
*— **Connor W. Coley**, Ye-Jin Hwang, Milad Abolhasani, Andreas L. Marzinzik, Guido Koch, Carsten Spanka, Hansjoerg Lehmann, Klavs F. Jensen*

8:40 Paper 507c: Ultrahigh-Throughput Screening of Chemical Synthetic Pathways Using Desorption Electrospray Ionization Mass Spectrometry *— **Andy Koswara**, Botond Szilagyi, Bradley P. Loren, Larissa V. Avramova, Christina E. Ferreira, Tiago JP Sobreira, Michael Wleklinski, Caitlin E. Falcone, Zinia Jaman, Harrison S. Ewan, Ryan T. Hilger, R. G. Cooks, David H. Thompson, Zoltan K. Nagy*

9:00 Paper 507d: Heuristics for Implementing Photoredox Catalysis in Flow Reactors *— **Eric G. Moschetta**, Steve Richter, Steven J. Wittenberger*

9:20 Paper 507e: Operando Raman of the Nitroaldol Reaction over Pore-Expanded FDU-12–Dendron Hybrids *— **Daniel Shantz**, Junxing Han*

9:40 Paper 507f: Scale-Up of a Reaction Step from Lab to Commercial Scale, Switching from Batch to Continuous Manufacturing Using a Mechanistic Modelling Approach *— **Filipe Ataíde**, Rudi Oliveira, Ruth Morais*

10:00 Paper 507g: Microreactors Driven by Electric Field for Enzyme Catalysis in ATPS
*— Alexandr Romanov, Lucie Vobecka, Zdenek Slouka, **Michal Pribyl***

(508) Recent Advances in Molecular Simulation Methods II
Wednesday, Nov 1, 8:00 AM
MCC, L100H

Erik E. Santiso, Chair
Cameron F. Abrams, Co-Chair
Harish Vashisth, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

8:00 Paper 508a: Elucidating Molecular Details of Protein Liquid-Liquid Phase Separation by a Coarse-Grained Model *— **Gregory L. Dignon**, Wenwei Zheng, Robert Best, Jeetain Mittal*

8:19 Paper 508b: Real-Time Electron Dynamics of Large Complex Systems from a Density-Functional Tight-Binding Approach *— **Bryan M. Wong***

8:38 Paper 508c: Computational Investigation of Ionic Liquids Nanostructure Formation at Mesoscale
*— **Sergiy Markutsya**, Justin B. Haskins, John W. Lawson*

8:57 Paper 508d: Ultra-Coarse-Grained Modeling of ATP Hydrolysis in an Actin Filament *— **Harshwardhan H. Katkar**, Aram Davtyan, Aleksander E. P. Durumeric, Glen M. Hocky, Gregory A. Voth*

9:16 Paper 508e: Validation of Biomolecular Force Fields Regarding Structural and Thermodynamic Properties of Cyclodextrins and Their Complexes *— **Julia Gebhardt**, Daniel Markthaler, Niels Hansen*

9:35 Paper 508f: Optimal Probes: A Machine Learning Platform for Design of Experimental Probes for Protein Dynamics *— **Diwakar Shukla**, Shriyaa Mittal*

9:54 Paper 508g: Deep Learning and Atomistic Simulations in High-Throughput Material Discovery
*— **Amir Barati Farimani***

10:13 Paper 508h: Advancing Molecular Simulation Methods with Machine Learning
*— **Johannes Hachmann***

(509) Renewable Hydrogen Production
Wednesday, Nov 1, 8:00 AM
MCC, 200C

Dushyant Shekhawat, Chair
Scott McWhorter, Co-Chair
Daniel J. Haynes, Co-Chair

Sponsored by: Advances in Fossil Energy R&D

8:00 Paper 509a: Conceptual Design and Techno-Economic Analysis of a Solar Hybrid Sulfur Process
*— **Maximilian B. Gorensek**, Claudio Corgnale, William A. Summers*

8:22 Paper 509b: Potential Size of and Value Proposition for H2@Scale Concept *— **Mark Ruth**, Paige Jadun, Amgad Elgowainy, Bryan S. Pivovar*

8:44 Paper 509c: An Overview of H2@Scale: Energy System-Wide Benefits of Increased H2 Implementation
*— **Bryan S. Pivovar***

9:06 Paper 509d: Highly Efficient Visible-Light Photocatalytic Production of H_2 *— **Yun Hang Hu***

9:28 Paper 509e: Dynamic Simulation of a Solar-Powered Hybrid Sulfur Process for Hydrogen Production
*— Maxmilian Gorensek, John Weidner, Claudio Corgnale, Tom Stanford, Satwick Boddu, Evan Smith, Zhuhair Al Lawati, **Edward P. Gatzke***

9:50 Paper 509f: Hydrogen Generation from Hydrogen Sulfide Decomposition
*— **Ryan J. Gillis**, Khalid A. Al Ali, William H. Green*

10:12 Paper 509g: Adsorptive On-Board Desulfurization of Liquid Fuels: High Efficiency in Desulfurization and Full Thermal Regeneration via Hot Exhaust Gas *— **Raphael Neubauer**, Norbert Kienzl, Christoph Hochenauer*

(510) Theory, Modeling and Simulation of Nuclear Chemical Processes
Wednesday, Nov 1, 8:00 AM
MCC, 200D

Valmor de Almeida, Chair
Maximilian B. Gorensek, Co-Chair

Sponsored by: Nuclear Engineering Division

8:00 Paper 510a: A Multi-Phase Continuum Approach to Modeling the Performance of a Fluidized-Bed Nuclear Reactor
*— **Maureen A. Howley**, S. Aghara*

8:22 Paper 510b: Large-Scale Atomistic Simulations of Low-Energy Helium Implantation into Tungsten Single Crystals *— **Karl D. Hammond**, Sophie Blondel, Lin Hu, Dimitrios Maroudas, Brian D. Wirth*

8:44 Paper 510c: Development of Electrochemical Process Models for Treatment of Used Nuclear Fuel
*— **Candido Pereira***

9:06 Paper 510d: Managing Spent Fuel Resources: Closing the Loop
*— **S. Aghara***

9:28 Paper 510e: Modeling of Nano-Fuzz Formation in Helium-Ion-Irradiated Tungsten
*— **Dwaipayan Dasgupta**, Karl D. Hammond, Lin Du, Dimitrios Maroudas, Brian D. Wirth*

9:50 Paper 510f: Modeling Xenon Transport in Molten Salt-Fueled Reactors *— **Valmor F. de Almeida**, Benjamin S. Collins, Robert K. Salko, Robert Z. Taylor*

10:12 Paper 510g: Vapor–Liquid Phase Equilibrium Diagram for Uranium Hexafluoride (UF6) Using Simplified Temperature-Dependent Intermolecular Potential Parameters (TDIP)
*— Ali Al-matar, **Housam Binous***

(511) Thermodynamics of Biomolecular Folding and Assembly
Wednesday, Nov 1, 8:00 AM
MCC, L100I

Sapna Sarupria, Chair
Andrew L. Ferguson, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

8:00 Paper 511a: Computational Study of the Stability of the Miniprotein Trp-Cage in Extreme Environments
*— **Betul Uralcan**, Sang Beom Kim, Pablo G. Debenedetti*

8:15 Paper 511b: Engineering Robust Activity in Extremophilic Enzymes
*— **Siva Dasetty**, Weigao Wang, Mark Blenner, Sapna Sarupria*

8:30 Paper 511c: Effect of Manufacturing Conditions on the Fabrication of Protein/Polysaccharide Biocompatible Nanotubes (BNTs)
*— **Luis F. Maldonado**, Jozef Kokini*

8:45 Paper 511d: Towards a Thermodynamic Model for Predicting Coiled-Coil Protein Structures
*— **Mojtaba Jokar**, Korosh Torabi*

9:00 Paper 511e: Effect of Residual Secondary Structure Propensity on Liquid-Liquid Phase Separation of TDP-43 *— **Gregory L. Dignon**, Gul H. Zerze, Nicolas Fawzi, Young C. Kim, Jeetain Mittal*

9:15 Break

9:30 Paper 511f: Solvation Contribution to the Conformational Preferences of the Hydrated Peptides
*— **Gul H. Zerze**, Alexander Bourque, Jeetain Mittal*

9:45 Paper 511g: Influence of Backbone Hydrogen Bonding on the Stability of the WW Domain of the Protein PIN1 *— **Daniel Markthaler**, Niels Hansen*

10:00 Paper 511h: Molecular Simulations of the Force Spectroscopy of a Biomimetic Polymer
*— **Aviel Chaimovich**, Christian Leitold, Christoph Dellago*

10:15 Paper 511i: Insights into the Binding of β-Wrapins to Amyloidogenic Proteins Using Simulations and Experiments *— **Asuka A. Orr**, Michael M. Wördehoff, Hamed Shaykhalishahi, Ewa A. Mirecka, Sai Vamshi R. Jonnalagadda, Wolfgang Hoyer, Phanourios Tamamis*

(512) Thermophysical Properties and Phase Behavior III: Complex Molecules and Mixtures
Wednesday, Nov 1, 8:00 AM
MCC, L100J

Amir Haji-Akbari, Chair
Harish Vashisth, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

8:00 Paper 512a: Monte Carlo Simulations Probing Interfacial Adsorption and Uptake in Surfactant Bilayers *— **J. Ilja Siepmann**, Mona Minkara, Jingyi Chen, Cor J. Peters*

8:20 Break

8:40 Paper 512c: Phase and Interfacial Behaviour of Aqueous-Two Phase Systems Based on Hyperbranched Polymers *— Andres Kulaguin Chicaroux, **Tim Zeiner***

9:00 Paper 512d: From Metallic Hydrogen to Polymeric Sulfur: Peculiar Thermodynamics of Polyamorphic Fluids *— **Lauren E. Amrhein**, Mikhail A. Anisimov, Frédéric Caupin, Michal Duška, Amanda Rosenbaum*

9:20 Paper 512e: Computational Studies of Mixtures of Refrigerants, Ionic Liquids and Deep Eutectic Solvents for Absorption Refrigeration Systems *— **Rubaiyet Abedin**, Sharareh Heidarian, John C. Flake, Francisco R. Hung*

9:40 Paper 512f: Oil Desulfurization Using Deep Eutectic Solvents via Liquid-Liquid Extraction *— Samah E. E. Warrag, Nerea R. Rodriguez, Martin Van Sint Annaland, Maaike C. Kroon, **Cor J. Peters***

10:00 Paper 512g: Relevance of Thermophysical Property Data in Rate-Based Gas Treating Simulations
*— **Diego E. Cristancho**, Jacob M. Crosthwaite, Allen Day, John Dowdle, Clare Worley*

10:20 Paper 512h: Identification of the Equilibrium Parameters for the Modeling of the Hydrogen Solubility in Heavy Crude Cuts Using the MATLAB-Aspen Connection *— **Camilo Monroy-Peña**, **Johana Orjuela***

(513) Topical Plenary: Chemical Engineers in Medicine III (Invited Talks)
Wednesday, Nov 1, 8:00 AM
MCC, 202A/B

Swomitra Mohanty, Chair
Leonard F. Pease III, Co-Chair

Sponsored by: Chemical Engineers in Medicine

8:00 Paper 513a: Neuronal Biosensors *— **Bernard Van Wie***

8:40 Paper 513b: Mix (and Unmix) It Up with Biomembranes *— **Margie Longo***

9:20 Paper 513c: Bridging the Gap Between Viral and Nonviral Gene Vectors *— **Josh Ramsey***

(514) Water Treatment, Desalination, and Reuse I
Wednesday, Nov 1, 8:00 AM
MCC, M100H

Isabel Escobar, Co-Chair
William Phillip, Co-Chair
Mahdi Malmali, Co-Chair

Sponsored by: Membrane-Based Separations

8:00 Paper 514a: Selective Desalination of Brackish Water by Electrodialysis for Irrigation Use
*— **Ben Cohen**, Naftali Lazarovitch, Jack Gilron*

8:20 Paper 514b: N-Nitrosodimethylamine (NDMA) Removal by Thin-Film Composite Polyamide Reverse-Osmosis Membranes *— **Adel Soroush**, Henry Croll, Santiago Romero-Vargas Castrillon*

8:40 Paper 514c: Reaction Kinetics for Microcystin-LR Degradation by Ozonation in a Basic Medium
*— **Joyner Eke**, Andrew Bleha, Priyesh Wagh, Isabel Escobar*

9:00 Paper 514d: Novel Cylindrical Cross-Flow Hollow Fiber Membrane Module for Direct-Contact Membrane Distillation–Based Desalination
*— Dhananjay Singh, Lin Li, Gordana Obuskovic, John Chau, **Kamalesh K. Sirkar***

9:20 Paper 514e: A Novel Process for Concurrent Desalination and Boron Removal *— Süer Kürklü, Sadiye Halitoglu-Velioglu, M. Göktug Ahunbay, S. Birgül Tantekin-Ersolmaz, **William B. Krantz***

9:40 Paper 514f: Condition Optimization for the Fabrication of Desalination Thin-Film Composite Membranes *— **Mohammed Kadhom**, Baolin Deng*

10:00 Paper 514g: Scale-Up of RO and UF Membrane Surface Nano-Structuring with Hydrophilic Polymer Brush Layers: Evaluation of Uniformity of Membrane Performance
*— **Soomin Kim**, Jie Zhang, Anditya Rahardianto, Yoram Cohen*

(515) Young Faculty Forum (Invited Talks)
Wednesday, Nov 1, 8:00 AM
MCC, 205D

Kevin J. Cash, Co-Chair
Reginald E. Rogers Jr., Co-Chair

Sponsored by: Young Faculty Forum

8:00 Paper 515a: Teaching as a Young Faculty Member — ***Matthew Cooper***

8:30 Paper 515b: Research as a Young Faculty Member — ***Markita Landry***

9:00 Paper 515c: Starting a Research Program at an R3 University — ***Eric Jankowski***

9:30 Paper 515d: Panel Discussion: Funding Your Research — *Reginald E. Rogers Jr., Kevin J. Cash,* ***Jean W. Tom, T. J. Mountziaris, Jung-Sheng Wu***

10:15 Paper 515e: Meet and Greet: Young Faculty Forum — ***Reginald E. Rogers Jr., Kevin J. Cash***

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(516) Electrokinetics: Advancing the Fundamentals
Wednesday, Nov 1, 9:00 AM
Hilton, Marquette IV/V/VI/VII

Adrienne Minerick, Chair
Sagnik Basuray, Co-Chair

Sponsored by:
2017 Annual Meeting of the AES Electrophoresis Society

9:00 Paper 516a: Entropic Trapping During DNA Transport in Microfluidic Gel Electrophoresis: A Monte Carlo Simulation — ***Sourav Bandyopadhyay****, Victor M. Ugaz*

9:15 Paper 516b: Obstacle-Density Effects on Particle Trapping in Insulator-Based Dielectrophoresis Systems — *Victor H. Perez-Gonzalez,* ***Roberto C. Gallo-Villanueva****, Blanca H. Lapizco-Encinas*

9:30 Paper 516c: Investigating the Impact of Low-Concentration Surfactant on Red Blood Cell Dielectrophoretic Responses — ***Sanaz Habibi****, Hector Moncada-Hernandez, Adrienne Minerick*

9:45 Paper 516d: Modeling of Nano-EIS in a High-Peclet-Number Packed Microfluidic Biosensor — ***Mehnaz Mursalat****, Natalija Tasovac, Sagnik Basuray*

10:00 Paper 516e: AC Electrohydrodynamics of Polarized Laminar Flows — ***Nicholas Mavrogiannis****, Zachary R. Gagnon*

10:15 Paper 516f: Electrophoresis-Based Separation of DNA in Non-Templated vs. Liposome-Nanotemplated Agarose Gel: A Search to Design Transport Characteristics for Tissue Engineering Scaffold — ***Dipendra Wagle****, J. Robby Sanders, Pedro E. Arce*

10:30 Paper 516g: Micro Electrokinetic Turbulence and Its Measurement in a Microchannel — ***Wei Zhao****, Fang Yang, Guiren Wang*

10:45 Paper 516h: Thermodynamic Modeling of Electrodes and Mobile Ions in Capacitive Deionization Cell Units with eNRTL Model — ***Yue Yu****, Chau-Chyun Chen*

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(517) John M. Prausnitz AIChE Institute Lecture
Wednesday, Nov 1, 11:15 AM
MCC, Ballroom B

Sipho C. Ndlela, Chair

Sponsored by: Awards Committee

11:15 Paper 517a: Process Systems Engineering Contributions in Pharmaceuticals — ***G. V. Rex Reklaitis***

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(518) ABET Updates and Insights (Invited Talks)
Wednesday, Nov 1, 12:30 PM
MCC, 205C

Randy S. Lewis, Co-Chair
Douglas K. Ludlow, Co-Chair
Troy Vogel, Co-Chair

Sponsored by:
Undergraduate Education

12:30 Paper 518a: ABET Updates and Insights — ***Douglas K. Ludlow****, Randy S. Lewis, Troy Vogel*

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(519) Adsorbent Materials for Sustainable Energy and Chemicals
Wednesday, Nov 1, 12:30 PM
MCC, M100F

Sunho Choi, Chair
Praveen Bollini, Co-Chair

Sponsored by:
Adsorption and Ion Exchange

12:30 Paper 519a: Recovery of Inorganic Phosphorus via Metal-Exchanged ZSM-5 — ***Michael J. Manto****, Pengfei Xie, Mitchell A. Keller, Wilhelm E. Liano, Tiancheng Pu, Chao Wang*

12:47 Paper 519b: Metal-Organic Framework for Subsequent/ Simultaneous Removal of CO_2 and H_2S from Natural Gas and Biogas — ***Youssef Belmabkhout***

1:04 Paper 519c: Metal-Organic Frameworks with High Volumetric Hydrogen Storage Capacities — ***Justin Purewal****, Michael Veenstra, Donald J. Siegel, Adam J. Matzger, Yiyang Liu, Alauddin Ahmed, Antek G. Wong-Foy*

1:21 Paper 519d: Three-Dimensional Lignin-Based Smart Aerogel for Controllable Oil/Water Separation — ***Jingxian Jiang****, Qinghua Zhang, Xiaoli Zhan, Fengqiu Chen*

1:38 Paper 519e: Tunable Fabrication of Carbon Nanofibers from Renewable and Waste Resources for the Desulfurization of LPG — ***Efstratios Svinterikos****, Mohamed Al Marzouqi, Ioannis Zuburtikudis*

1:55 Paper 519f: Size-Controllable MOF Composite Particles for Bio-Butanol Recovery by Adsorption: Formulation and Mass Transfer Resistances — ***Julien Cousin Saint Remi****, Stijn Van der Perre, Gino Baron, Joeri Denayer*

2:12 Paper 519g: Synthesis and Granulation of a Ca-X Zeolite-Based Molecular Sieve and Adsorption Equilibrium of Oxidative Coupling of Methane Gases — ***Hector D. Diaz Ortiz****, Alvaro Orjuela, Gerardo Rodriguez, Jens-Uwe Repke, Hamid Reza Godini*

2:29 Paper 519h: Development of Aminopolymer-Based Sorbents for CO_2 Capture with Improved Capacity and Oxidative Stability — ***Michele L. Sarazen****, Simon H. Pang, Christopher W. Jones*

2:46 Paper 519i: Experimental Studies of 4.6-Dimethyldibenzothiophene Adsorption on Metal-Exchanged Mesoporous Y Zeolites — ***Kevin X. Lee****, George Tsilomelekis, Julia A. Valla*

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(520) Advances in Dividing-Wall Towers
Wednesday, Nov 1, 12:30 PM
MCC, M100G

Daniel R. Summers, Chair
Clint P. Aichele, Co-Chair
Andrew W. Sloley, Co-Chair

Sponsored by:
Distillation and Absorption

12:30 Paper 520a: Scaling Up Dividing-Wall Distillation Columns — ***Bailee Roach****, R. Bruce Eldridge*

12:55 Paper 520b: Optimizing Dividing-Wall Distillation Columns — ***Colton Andrews****, Bailee Roach, R. Bruce Eldridge*

1:20 Paper 520c: Dividing-Wall Columns as Applied to FCC, Coker & CCR Gas Plants — ***Manish Bhargava***

1:45 Paper 520d: Improving Thermal Efficiency and CO_2 Emission of the Dividing-Wall Column — ***Md. Aurangzeb****, Amiya Kumar Jana*

2:10 Paper 520e: Design, Optimization and Control of Energy-Saving Dividing-Wall Column for Separating Azeotropes — ***Ming Xia****, Zhongyi Ma, Litao Jia, Bo Hou, Debao Li*

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(521) Advances in Life-Cycle Optimization for Process Development
Wednesday, Nov 1, 12:30 PM
MCC, 102F

Gonzalo Guillén-Gosálbez, Chair
Debalina Sengupta, Co-Chair
Jose Maria Ponce-Ortega, Co-Chair

Sponsored by: Process Development

12:30 Paper 521a: Greenhouse Gas Intensities and Energetic Productivity Dynamics of Giant Global Oilfields: A Life-Cycle Approach — ***Mohammad S. Masnadi****, Adam Brandt*

12:51 Paper 521b: Economic and Environmental Evaluation of Olive Mill Wastewater Treatment Methods for a Self-Supplied American Olive Oil Mill — ***Chae Woon Jeong****, Benjamin J. Davis*

1:12 Paper 521c: Systematic Generation of Hybrid Insulation Materials via Data Envelopment Analysis — ***Alba Torres Rivas****, Anna Ewertowska, Carlos Pozo, Dieter Boer Sr., Laureano Jiménez Esteller*

1:33 Paper 521d: Eco-Efficiency Assessment of EU Manufacturing Sectors Linking Multi-Regional Environmentally Extended Input-Output Tables and Data Envelopment Analysis — ***Gonzalo Guillén-Gosálbez****, Patricia Zurano-Cervello, Carlos Pozo, Laureano Jimenez, Jose Maria Mateo-Sanz*

1:54 Paper 521e: Life-Cycle Optimization with Ecosystems as Unit Operations — ***Tapajyoti Ghosh,*** *Bhavik R. Bakshi*

2:15 Paper 521f: Techno-Economic Assessment of Dry Reforming of Methane Process — ***Shaik Afzal****, Debalina Sengupta, Mahmoud El-Halwagi, Nimir Elbashir*

2:36 Paper 521g: Coupling the P-Graph Framework with Life-Cycle Assessment: Process Synthesis of Biofuels and Biochemicals Co-Production for Environmental Performance — ***Andrew Beck****, George G. Zaimes, Vikas Khanna*

(522) Advances in MINLP and Global Optimization
Wednesday, Nov 1, 12:30 PM
MCC, 103E

Kamil A. Khan, Chair
Nihar Sahay, Co-Chair

Sponsored by:
Computers in Operations and Information Processing

12:30 Paper 522a: Global Optimization of Nonconvex Problems with Convex-Transformable Intermediates — ***Carlos Nohra****, Nick Sahinidis*

12:51 Paper 522b: Deterministic Global Optimization Algorithm Using Piecewise Relaxations and Bound Tightening with Dynamic Partitioning — ***Pedro A. Castillo Castillo****, Pedro M. Castro, Vladimir Mahalec*

1:12 Paper 522c: A Level-Based Quadratic Outer Approximation Algorithm for Convex MINLP — ***Jan Kronqvist****, David E. Bernal, Ignacio E. Grossmann*

1:33 Paper 522d: Heuristic for Improved McCormick Relaxations in a Branch-and-Bound Framework — *Jaromił Najman,* ***Alexander Mitsos***

1:54 Paper 522e: Scalable Global Algorithms for Stochastic Nonlinear Programming — *Victor M. Zavala,* ***Yankai Cao***

2:15 Paper 522f: Analysis of the Alternating Direction Method of Multipliers for the Optimization of Distributed Nonconvex Systems — ***Stuart Harwood****, Shivakumar Kameswaran, Thomas A. Badgwell*

2:36 Paper 522g: Guaranteed Global Optimization of Expected-Value Minimization Problems with Continuous Random Variables — *Yuanxun Shao,* ***Joseph Scott***

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(523) Advances in Protein Expression, Post-Translational Modification and Biomanufacturing
Wednesday, Nov 1, 12:30 PM
MCC, 206A/B

Adam Melvin, Chair
Kang Wu, Co-Chair

Sponsored by: Bioengineering

12:30 Paper 523a: Modulating Antibody/Antigen Affinity by Triggered Assembly and Disassembly of an Artificially Split Protein M — *Heejae Kim,* ***Andrew Gaynor****, Wilfred Chen*

12:48 Paper 523b: Systems Engineering N-Glycans of Recombinant Therapeutic Proteins Produced in Mammalian Cells — ***Meghan G. McCann****, Tung S. Le, Christopher Stach, Xinning Chen, Nikunj Somia, Liang Zhao, Michael J. Smanski, Wei-Shou Hu*

1:06 Paper 523c: A Framework for Development of Integrated and Computationally Feasible Models of Large-Scale Mammalian Cell Bioreactors — ***Parham Farzan****, Marianthi Ierapetritou*

1:24 Paper 523d: Multi-Enzyme Display on Bacterial Spore Surface for Plastic Degradation — *Erin Drufva,* ***Kang Wu***

1:42 Paper 523e: Posttranslational Modifications as Regulators of Activity in Nucleus Versus Mitochondria — ***Lawrence I. Grossman****, Neeraja Purandare, Stephanie Gladyck, Mallika Somayajulu, Maik Hüttemann, Siddhesh Aras*

2:00 Paper 523f: Location-Dependent Effect of Post-Translational Pegylation on Pegylation Efficiency and the Activity and Protein Stability of T4 Lysozyme — ***Kristen M. Wilding****, Bradley C. Bundy*

2:18 Paper 523g: Making Water-Soluble Integral Membrane Proteins Directly in Living Cells — ***Matthew Delisa***

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(524) Amorphous and Crystalline Particle Engineering in Pharmaceuticals and Other Novel Materials
Wednesday, Nov 1, 12:30 PM
MCC, M100J

Gaurav Giri, Chair
Meenesh R. Singh, Co-Chair
Jason Sweeney, Co-Chair

Sponsored by:
Crystallization and Evaporation

12:30 Introductory Remarks

12:35 Paper 524a: Understanding and Controlling Organic Molecule and Metal-Organic Framework Crystallization — ***Gaurav Giri***

12:55 Paper 524b: Design of API Amorphous Precipitation Processes via the Use of an FBRM-Based Method — ***Eric Sirota****, Dimitrios Zarkadas*

1:15 Paper 524c: Spray-Dried Particle Formation Model to Predict Application Performance — ***Jaime Curtis-Fisk****, Priti Jain, Shrikant Khot, William Porter III*

1:35 Paper 524d: Facile Synthesis of Soft-Templated Carbon Nitrides with High Surface Area and Porosity — ***Marcella Lusardi****, Maryam Peer, Klavs F. Jensen*

1:55 Paper 524e: Production of Large Quantities of ZIF-8 Through Batch- and Semi-Continuous Processes — ***Stoner Josie****, Gerold A. Willing, John L. Tatarko Jr.*

2:15 Paper 524f: Study of Silica Precipitation in a Hydrometallurgical Process — ***Christian Manfoumbi****, Martine Meireles Masbernat*

2:35 Paper 524g: Separation of Isomers — ***Patrick Zimmermann****, Thomas Goetsch, Sabine Enders, Tim Zeiner*

2:55 Concluding Remarks

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(525) Biomaterials for Drug Delivery I: Particle-Based Drug Delivery
Wednesday, Nov 1, 12:30 PM
MCC, 209A/B

Mathumai Kanapathipillai, Chair
Lei Zhang, Co-Chair

Sponsored by: Biomaterials

12:30 Break

1:06 Paper 525c: TAT-Functionalized Liposomes for the Treatment of Meningitis — ***Caterina Bartomeu Garcia****, Di Shi, Thomas J. Webster*

1:24 Paper 525d: Cartilage-Penetrating Nanoparticles to Provide Sustained Delivery of Disease-Modifying Drugs in Post-Traumatic Osteoarthritis — ***Brett C. Geiger****, Sheryl Wang, Alan Grodzinsky, Paula T. Hammond*

1:42 Paper 525e: Nanoparticle Tracking Analysis of Polymer Particle Aggregation in Blood Plasma — ***Kathleen McEnnis****, Stephanie Christau, Sean McLoughlin, Joerg Lahann*

2:00 Paper 525f: High-Throughput Screening of Biodegradable Nanogels with Tunable Size and Swelling for Intracellular Drug Delivery — ***David S. Spencer****, Bryan C. Luu, David W. Beckman, Nicholas A. Peppas*

2:18 Paper 525g: Polyanhydride Nanoparticles Encapsulating Rifampicin Suppress Growth of Pathogenic Acanthamoeba In Vitro — ***Nathan Peroutka-Bigus****, Adam Mullis, Balaji Narasimhan, Bryan H. Bellaire*

2:36 Paper 525h: Design of Dual-Encapsulated Biodegradable Nanoparticles for Cancer Treatment — ***Amber C. Jerke****, Timothy M. Brenza*

(526) Biomaterials for Immunological Applications I: Immune Activation and Vaccination
Wednesday, Nov 1, 12:30 PM
MCC, 211A

Bret Ulery, Chair
R. Michael Gower, Co-Chair
Peipei Zhang, Co-Chair

Sponsored by: Biomaterials

12:30 Paper 526a: Understanding How Lipid Nanoparticle Structure Affects Immune Response — ***Lisa Kasiewicz****, Sushant Kumar, Rahul Purwar, Kathryn A. Whitehead*

12:48 Paper 526b: Multi-Stage Drug Delivery System for Enhanced Payload Delivery to Lymph Node Cells — ***Alex Schudel****, Cody Higginson, Mai Kwan Yau, M. G. Finn, Susan N. Thomas*

1:06 Paper 526c: Encapsulation and Thermal Stability of Immunological Biologics Using Complex Coacervation — ***Whitney C. Blocher****, Rebecca Hershman, Sarah L. Perry*

1:24 Paper 526d: Evaluation of Biocompatibility of Novel Block Copolymer Gels/Micelles as Potential Vaccine Adjuvants — *Justin Adams,* ***Sujata Senapati****, Michael J. Wannemuehler, Balaji Narasimhan, Surya Mallapragada*

1:42 Paper 526e: Intranasal Nanovaccine Provides Protection Against Homologous and Heterologous Influenza Virus — *Zeb Zacharias,* ***Kathleen Ross****, Balaji Narasimhan, Thomas Waldschmidt, Kevin Legge*

2:00 Paper 526f: Design of a Combination Nanovaccine to Induce Rapid and Long-Term Protective Immunity Against Bacillus anthracis — ***Sean Kelly,*** *Ross Darling, Nathan Peroutka-Bigus, Thomas Dubensky, Bryan H. Bellaire, Michael J. Wannemuehler, Balaji Narasimhan*

2:18 Paper 526g: Comprehensive Vaccine Design for Commensal Disease Progression — *Charles H. Jones, Guojian Zhang, Roozbeh Nayerhoda,* ***Marie Beitelshees****, Andrew Hill, Yi Li, Bruce A. Davidson, Paul Knight III, Blaine Pfeifer*

2:36 Paper 526h: Oncofetal Antigen Peptide Nanoclusters for Cancer Vaccines — ***Alexandra Tsoras****, Julie A. Champion*

(527) Biomolecules at Interfaces II
Wednesday, Nov 1, 12:30 PM
MCC, M100B

Prajnaparamita Dhar, Chair
Susan Daniel, Co-Chair
Bernardo Yanez Soto, Co-Chair

Sponsored by: Interfacial Phenomena

12:30 Welcoming Remarks

12:33 Paper 527a: Molecular Perspective on Protein-Protein Interactions at the Tight Junctions Interface — ***Flaviyan Jerome Irudayanathan***, *Shikha Nangia*

12:49 Paper 527b: Pore Formation by Aggregates of Antimicrobial Peptides in DMPC Bilayers — *Yuan Lyu, Maya Frityanti, Xiao Zhu,* ***Ganesan Narsimhan***

1:05 Paper 527c: Single-Molecule Characterization of Protein Adsorption to Multivalent Glycan Polymers — *Bhargava Nemmaru, Sonia K. Brady, Matthew J. Lang,* ***Shishir P. S. Chundawat***

1:21 Paper 527d: Controlling Local Hydrophobicity in Poly(ethylene glycol) Brushes with Poly(sulfobetaine) to Mediate the Conformation of Fibronectin on Biomaterial Surfaces — ***David Faulón Marruecos***, *Hye Hyun Kim, Michael R. Shirts, Daniel K. Schwartz, Joel L. Kaar*

1:37 Paper 527e: Adsorption of Recombinant Human Interleukin-1 Receptor Antagonist to Silicone Oil-Water Interfaces Leads to Gel Formation and Subsequent Surface-Induced Aggregation — ***Lea L. Sorret***, *Theodore W. Randolph*

1:53 Paper 527f: Fibrinogen Adsorption onto Phospholipid Monolayers: Aging and Stiffening — ***Ian Williams***, *Todd M. Squires*

2:09 Paper 527g: Morphological and Mechanical Studies of Multicomponent Phospholipid Monolayers Containing 27-Hydroxycholesterol — ***Benjamin L. Stottrup***, *Amit Kumar Sachan, Joesph A. Zasadzinski*

2:25 Paper 527h: Understanding the Effect of Engineered Carbon Nanodiamonds on the Reversible Collapse of Lung Surfactant Monolayers — ***Aishik Chakraborty***, *Prajnaparamita Dhar*

2:41 Paper 527i: High-Resolution Optical and Electrical Recording of Free-Standing Lipid Bilayers — ***Peter J. Beltramo***, *Jan Vermant*

2:57 Concluding Remarks

(528) Catalysis for C1 Chemistry: Producing and Converting Methanol
Wednesday, Nov 1, 12:30 PM
MCC, L100D

Elizabeth J. Biddinger, Chair
Dolly Chitta, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

12:30 Paper 528a: Selective Oxidation of Methane to Methanol in Zeolites: A Window of Opportunity — ***Ambarish R. Kulkarni***, *Jens K. Nørskov, Felix Studt*

12:48 Paper 528b: Computational Screening and Characterization of Single-Site Active Porous Surface for Natural Gas-to-Liquid Feedstock Conversion Process — ***Pabitra Choudhury***, *Thalia Quinn, Joseph Kerwin, Sierra Headrick, Sean Mussell*

1:06 Paper 528c: Selective Oxidation of Methane to Methanol or Acetic Acid on Rhodium Single-Site Catalysts at Mild Conditions — ***Mengwei Li***, *Junjun Shan, Maria Flytzani-Stephanopoulos*

1:24 Paper 528d: Synergistic Effects Between CHA Zeotypes and Basic Metal Oxides in Bifunctional Strategies for Improved Lifetime in Methanol-to-Olefins Catalysis — ***Andrew Hwang***, *Aditya Bhan*

1:42 Paper 528e: Depressed Deactivation of SAPO-34 During Methanol-to-Olefins Process by MgO — ***Sheng-Li Chen***, *Ya Wang, Yu-Li Gao, Qi Zhang, Ying-qian Cao, Jay Benziger, Wei-Ke Chang*

2:00 Paper 528f: Investigating Alkene Formation Pathways in Methanol-to-Hydrocarbon Processes Within Zeolites — ***Pavlo Kravchenko***, *Mykela Deluca, David D. Hibbitts*

2:18 Paper 528g: Different Dependency on Copper Oxidation States Between H_2 and CO_2 Production During Partial Oxidation of Methanol — ***Hao Chi***, *Christopher M. Andolina, Jonathan Li, Matthew Curnan, Guangwen Zhou, Goetz Veser, Judith C. Yang*

(529) Catalysis for Pharmaceuticals and Fine Chemicals
Wednesday, Nov 1, 12:30 PM
MCC, L100B

Marimuthu Andiappan, Chair
Ali A. Rownaghi, Co-Chair
Steven R. Saunders, Co-Chair
Heather Mayes, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

12:30 Paper 529a: Regioselective Alcohol Ring Opening of Epoxides Using Lewis Acidic Catalysts — ***Nitish Deshpande***, *Aamena Parulkar, Rutuja Joshi, Nicholas Brunelli*

12:50 Paper 529b: Closed-Loop Multi-Target Optimization for Discovery of Chemical Reactions — *Alexander Echtermeyer,* ***Yehia Amar***, *Jacek Zakrzewski, Alexei Lapkin*

1:10 Paper 529c: Engineering Porous Polymer Hollow Fiber Microfluidic Reactors for Sustainable C-H Functionalization — ***Yingxin He***, *Ali A. Rownaghi*

1:30 Paper 529d: Comparison of Pd Catalyst Activation Protocols in Suzuki Coupling and Associated Impacts on In-Process Control and Process Performance — *Carolyn S. Wei, Ye Zhu, Lingfeng He,* ***Eric C. Huang***, *Brendan C. Mack, Thomas M. Razler, Christopher C. Wood*

1:50 Paper 529e: Plasmonic Catalysts as Efficient Catalysts for Cross-Coupling Reactions — ***Andishaeh Dadgar***, *Farshid Mohammadparast, Marimuthu Andiappan*

2:10 Paper 529f: Stereoconvergent Tandem Systems Combining Photocatalyzed Isomerization and Enzymatic Reduction for Chiral Building Blocks Synthesis — ***Yajie Wang***, *Zachary Litman, Huimin Zhao, John F. Hartwig*

2:30 Paper 529g: A Model-Based Approach for the Identification of Kinetic Models from Laboratory Reactors — ***Lu Han***

(530) Catalysis with Microporous and Mesoporous Materials IV
Wednesday, Nov 1, 12:30 PM
MCC, L100A

Viktor J. Cybulskis, Chair
Marat Orazov, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

12:30 Paper 530a: Acid-Catalyzed Production of 1,3-Butadiene from Biomass-Derived Tetrahydrofuran — ***Omar A. Abdelrahman***, *Dae Sung Park, Katherine Vinter, Charles S. Spanjers, Limin Ren, Hong Je Cho, Dion Vlachos, Wei Fan, Michael Tsapatsis, Paul J. Dauenhauer*

12:48 Paper 530b: External Surface and Pore Mouth Catalysis in Hydrolysis of Inulin over Zeolites with Different Micropore Topologies and Mesoporosities — ***Su Cheun Oh***, *Thien Nguyendo, Yao He, Amanda Filie, Yiqing Wu, Dongxia Liu*

1:06 Paper 530c: On the Role of Na Cations and Solvent in Glucose Isomerization and Epimerization in Sn-BEA — ***Sha Li***, *Tyler R. Josephson, Dionisios G. Vlachos, Stavros Caratzoulas*

1:24 Paper 530d: Liquid-Phase Propylene Epoxidation with Nb-Based Mesoporous Silicates — ***Swarup Maiti***, *Anand Ramanathan, Bala Subramaniam*

1:42 Paper 530e: Catalytic Activity of Unique Base Sites Formed via Nitridation and Subsequent Methylation of Mesoporous Silica SBA-15 — ***Takahiko Moteki***, *Masaru Ogura*

2:00 Paper 530f: The Effect of Water on the Reusability of Aminated Mesoporous Silica Catalysts for Aldol Condensations — ***Anton De Vylder***, *Jeroen Lauwaert, Jeriffa De Clercq, Pascal van Der Voort, Joris W. Thybaut*

2:18 Paper 530g: Novel Method for Synthesizing Non-Leaching Functionalized Mesoporous-Silica for Acid-Catalyzed Alkylation Reaction — *Daniel Resasco,* ***Tuong Bui***, ***Santiago Umbarila***

2:36 Paper 530h: Catalytic Conversion of Biomass-Derived Ethanol to Advanced Hydrocarbon Fuels and Valuable Chemicals — ***Zhenglong Li***, *Andrew W. Lepore, Mariam Salazar, Brian H. Davison, Chaitanya Narula*

(531) Cell Culture Engineering & Process Design II: Reactor Engineering
Wednesday, Nov 1, 12:30 PM
MCC, 208C/D

Nicholas Graham, Chair
Kang Zhou, Co-Chair

Sponsored by: Bioengineering

12:30 Paper 531a: Evaluation of the Impact of Viable Cell Density on kLa for Oxygen Transfer in Perfusion Bioreactors — ***Chun Chen***, *Gregory Frank, Neil Soice*

12:48 Paper 531b: Performance Characterization and Process Validation of a Mini-Scale Bioreactor for Recombinant Mammalian Cells — ***Cameron Bardliving***

1:06 Paper 531c: Improving Biocompatibility of 3D-Printed Stereolithography Resins — ***Christopher J. Hawxhurst***, *Andrea L. Kadilak, Charles M. Bridges, Daniel J. Gage, Leslie M. Shor*

1:24 Paper 531d: Monoclonal Antibody (mAb) Production in Continuous Microfluidic Systems — *Grissel Trujillo-de Santiago, Everardo González-González, Ricardo Hernández Medina, Claudia del Toro Runzer, Ali Khademhosseini,* ***Mario M. Alvarez***

1:42 Paper 531e: Application of Mass Transfer Modeling to Improve Predictability of Scale-Down Industrial Fermentation Processes — ***Heather Jones***, *Chris Stowers, Patrick Reifel*

2:00 Paper 531f: Enhanced Oxygen Transfer and Cell Growth in a Continuous Rotating Bioreactor — ***Shu Fang***, *Paul W. Todd, Thomas R. Hanley*

2:18 Paper 531g: Using Metabolic Modeling and Metabolomics to Improve Cell Culture-Based Bioprocesses — ***Kyongbum Lee***

(532) Characterization of Adsorbent Materials
Wednesday, Nov 1, 12:30 PM
MCC, M100E

Federico Brandani, Chair
Nicholas C. Burtch, Co-Chair

Sponsored by:
Adsorption and Ion Exchange

12:30 Paper 532a: How Reliable Are Isotherm Measurements in Metal-Organic Frameworks? — ***Jongwoo Park***, *Joshua D. Howe, David S. Sholl*

12:55 Paper 532b: Toolkit for a Reliable Characterization of Hierarchical Structured Nanoporous Materials by Physical Adsorption and Mercury Porosimetry — *Katie Cychosz,* ***Matthias Thommes***

1:20 Paper 532c: Temperature Dependence of CO_2 Sorption in Micro-Mesoporous Carbons — ***F. Silvio P. Dantas***, *Richard T. Cimino, Katie A. Cychosz, Matthias Thommes, Alexander V. Neimark*

1:45 Paper 532d: Pore Size Distribution in Hierarchical Materials: Insights from Molecular Simulations — ***Mansi S. Shah***, *Swagata Pahari, Limin Ren, Matthias Thommes, Michael Tsapatsis, J. Ilja Siepmann*

2:10 Paper 532e: Investigating Imine-Based Porous Organic Cage Formation Mechanisms Using Time-Resolved Mass Spectrometry and Quantum Chemical Calculations — ***Guanghui Zhu***, *Luis Flores, David A. Dixon, Christopher W. Jones, Ryan Lively*

(533) Chemical and Catalytic Conversions and Processes for Renewable Feedstocks
Wednesday, Nov 1, 12:30 PM
MCC, 101B

Justinus Satrio, Chair
Michael Mullins, Co-Chair

Sponsored by:
Sustainable Biorefineries

12:30 Paper 533a: Catalytic Upgrading of Biomass Derivatives to Renewable Jet Fuels — ***Basudeb Saha***, *Saikat Dutta*

12:55 Paper 533b: Continuous Hydrogenation of Furfural to Cyclopentanone Using Activated Carbon Monolith Catalysts — ***Maryam Pirmoradi***, *James Kastner, Robert J. Gulotty Jr.*

1:20 Paper 533c: Soluble Sugars from Cellulose Using Polyvinyl Chloride-Derived Hydrochloric Acid as Catalyst — ***Joel Braden***, *Yuan Xue, Patrick A. Johnston, Xianglan Bai*

1:45 Paper 533d: Effect of Temperature and Vapor Residence Time on Product Distribution of High-Density Polyethylene Fast Pyrolysis — ***Ulises R. Gracida-Alvarez***, *Mary Kate Mitchell, Julio C. Sacramento-Rivero, David R. Shonnard*

2:10 Paper 533e: Effects of Acid-Pretreatment on Co-Pyrolysis of Biomass and Plastic — ***Yuan Xue***, *Xianglan Bai*

2:35 Paper 533f: Effect of Dielectric Oxides on Microwave-Assisted Deconstruction of Lignin — ***Piyali Dhar***, *R. Vinu*

(534) Coal Conversion to Value-Added Chemicals and Power in Modular Systems
Wednesday, Nov 1, 12:30 PM
MCC, 101D

James C. Fisher II, Chair
Kunlei Liu, Co-Chair

Sponsored by:
Advances in Fossil Energy R&D

12:30 Paper 534a: Thermodynamic Simulations and Techno-Economic Analysis on the Utilization of CO_2 and a Novel Modularization Strategy for Chemical Looping–Based GTL Processes — ***Mandar Kathe***, *Peter Sandvik, Charlie Fryer, Frank Kong, Abbey Empfiled, Liang-Shih Fan*

12:48 Paper 534b: Catalytic PRB Coal-CO_2 Gasification for Producing Syngas with Almost Zero CH_4 and Desired H_2:CO Ratio Required for Chemical and Fuel Synthesis — ***Wenyang Lu***, *Qinxi Cao, Bang Xu, Maohong Fan*

1:06 Paper 534c: Gasification of Residue from the Solvent Extraction of Powder River Basin Coal — *William C. Schaffers, Ying Wang,* ***David A. Bell***

1:24 Paper 534d: Development of a Modular Coal/Biomass to Fischer-Tropsch Liquids Research Facility — ***Andrew Placido***, *Kunlei Liu*

1:42 Paper 534e: Microwave-Assisted Pyrolysis of Coals and Coal Blends of Different Origin for Liquid and Solid Fuel Production — ***Rajasekhar Reddy Busigari***, *R. Vinu*

2:00 Paper 534i: Production of fuels from coal-biomass feedstock using Fischer-Tropsch — ***Burtron H. Davis***

2:18 Paper 534g: Coal Power Plants with Enhanced Profitability and No Carbon Dioxide Emissions — ***Chuanjun Jiao***, *Vasilios Manousiouthakis*

2:36 Paper 534h: Red Mud Catalyst for Tar-Free Syngas Production for Higher-Value Applications — ***Foster Agblevor***, *Oleksandr Hietsoi, Francine Battaglia*

(535) Complex Fluids: Self & Directed Assembly
Wednesday, Nov 1, 12:30 PM
Hilton, Conrad D

Subramanian Ramakrishnan, Chair
Simon Rogers, Co-Chair

Sponsored by: Fluid Mechanics

12:30 Paper 535a: Dynamics of Lipid Lamellae and Lamellar Vesicles in Shear and Extensional Flows — *Subas Dhakal,* ***Radhakrishna Sureshkumar***

12:45 Paper 535b: Probing the Structure of High-Viscosity Complex Fluids at High Shear Rates — ***Javen Weston***, *Kathleen Weigandt, Steven D. Hudson*

1:00 Paper 535c: Mechanistic Constitutive Model for Wormlike Micelle Solutions with Flow-Induced Structure Formation — *Sarit Dutta,* ***Michael Graham***

1:15 Paper 535d: Rheology and Microstructure of Thermoreversible Micellar Crystals in Ionic Liquid — ***Ru Chen***, *Carlos R. López-Barrón, Norman J. Wagner*

1:30 Paper 535e: Use of Microfluidics and Advanced Microscopy to Study Shear-Induced Structuring in Wormlike Micellar Solutions — ***Carla Caiazza***, *Valentina Preziosi, Giovanna Tomaiuolo, Denis O'Sullivan, Vincenzo Guida*

1:45 Paper 535f: A Multiscale Tensor-Based Model for the Rheology of Aggregating Thixotropic Colloidal Suspensions — *Paul M. Mwasame,* ***Antony N. Beris***, *Norman J. Wagner*

2:00 Paper 535g: Effect of Shear Stress on Rheological Properties of Fibrous Colloidal Gels During Gel-Sol Transitions Induced by Osmotic Pressure Gradients — ***Matthew Wehrman***, *Seth Lindberg, Kelly M. Schultz*

2:15 Paper 535h: Microstructural Basis for Colloidal Gel and Glass Aging — ***Melissa B. Gordon***, *Christopher J. Kloxin, Norman J. Wagner*

2:30 Paper 535i: The Mechanism for Shear Thickening in Viscoelastic Suspensions — ***Mengfei Yang***, *Eric S. G. Shaqfeh*

2:45 Paper 535j: Homogenization of Self-Organizing Colloidal Particles in a Microscopy Chamber — ***Paul W. Todd***, *Michael (Andy) Kurk, Scott Moyers*

(536) Composites for Environmental Applications
Wednesday, Nov 1, 12:30 PM
MCC, 211D

Evan K. Wujcik, Chair
Sitaraman Krishnan, Co-Chair
Lichen Xiang, Co-Chair
Gang Wu, Co-Chair

Sponsored by: Composites

12:30 Paper 536a: S-Doped TiO_2 for Photocatalytic Oxidation of CO in Visible Region Synthesized by Novel One-Step Liquid Flame Spray Pyrolysis (LFSP): Kinetics and Mechanism — ***Siva Nagi Reddy Inturi***, *Panagiotis Smirniotis*

12:47 Paper 536b: Copper Hexacyanoferrate Hydrogel Electrodes for Electrochemically Mediated Cation Separations — ***Kai-Jher Tan***, *Xiao Su, Johannes Elbert, T. Alan Hatton*

1:04 Paper 536c: Emulsion-Templated Polymers as Structured Supports for MOF Adsorbents — ***Jacob I. Deneff***

1:21 Paper 536d: Development of Novel Crosslinked Polymers for the Capture of Environmental Pollutants — ***Rishabh Shah***, *Thomas Dziubla, J. Zach Hilt*

1:38 Paper 536e: Grafted Polystyrene-Controlled Formation of Magnetic Carbon Nanocomposites for Environmental Remediation — ***Hongbo Gu***

1:55 Paper 536f: Constructing Fenton-Like Reaction over g-C_3N_4/NH_2-MIL-88B(Fe) Photocatalyst to Degrade Organic Contamination in Aqueous Solution — ***Xiyi Li***, *Yunhong Pi,* ***Zhong Li***, ***Jing Xiao***

2:12 Paper 536g: Synthesis of Thermoresponsive Composite and Application for Water Treatment
— ***Junichi Ida***, *Masanori Ochi, Ai Ishikawa, Atsushi Matsumoto, Tatsushi Matsuyama, Hideo Yamamoto*

2:29 Paper 536h: Integrated Adsorption and Visible-Light-Driven Photocatalytic Degradation of MB over Oxidized C_{60}/NH_2-MIL68(In)
— ***Yunhong Pi***, *Xiyi Li, Zhong Li, Jing Xiao*

2:46 Paper 536i: In-Situ Studies on Anion Electroadsorption Mechanisms
— ***Kelsey Hatzell***, *Marta Hatzell, Marm Dixit*

(537) Computational Catalysis III: Electrocatalysis
Wednesday, Nov 1, 12:30 PM
MCC, L100E

Bin Wang, Chair
Ronald Michalsky, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

12:30 Paper 537b: Saddle Point Searches in Electrochemical Reactions
— ***Per Lindgren***, *Georg Kastlunger, Muammar El Khatib, Andrew A. Peterson*

1:00 Paper 537d: Enhanced Activity for Oxygen Reduction Reaction by Gold at Step/Edge Sites of Ni@Aupt Core-Shell Nanoparticles: A DFT Investigation
— ***Wei An***, *Hao Wang*

1:30 Paper 537f: Ammonia Synthesis Using Plasma-Assisted Catalysis: Understanding Rate Enhancements by Excited Species — ***Prateek Mehta***, *Jongsik Kim, David Go, Jason C. Hicks, William F. Schneider*

2:00 Paper 537h: An Importance of Ligand Effects Breaking the Scaling Relation for Core-Shell Oxygen Reduction Catalysts — ***Seoin Back***, *Yousung Jung*

(538) Conjugated Polymers
Wednesday, Nov 1, 12:30 PM
MCC, 211C

Allie Obermeyer, Chair
Ying Diao, Co-Chair
Rafael Verduzco, Co-Chair

Sponsored by: Polymers

12:30 Paper 538a: Engineering Materials and Processes for Flexible Electronics — ***Antonio Facchetti***

1:00 Paper 538b: Spectroelectrochemistry of Conjugated Radical Polymers
— ***Jodie L. Lutkenhaus***

1:15 Paper 538c: Conjugated Copolymers Based on Purines: Linking Monomer Design and Macromolecular Properties — ***Michael Kilbey***, *Graham Collier, Lauren Brown, Evan Boone, Brian Long*

1:30 Paper 538d: "Greener" Synthesis of p-Conjugated Organic Semiconductors via Direct C-H Arylation Coupling — ***Mingfeng Wang***

1:45 Paper 538e: Pinch-Off Dynamics and Printability of Semi-Flexible and Rigid Rod Polymer Solutions
— *Leidy N. Jimenez, Jelena Dinic,* ***Vivek Sharma***

2:00 Paper 538f: Surface-Directed Multiscale Assembly of Conjugated Polymers — ***Ying Diao***, *Erfan Mohammadi, Ge Qu*

2:15 Paper 538g: Interpenetrating Networks for Flexible Bulk Heterojunction OPVs — ***Jorge Mok***, *Zhiqi Hu, Rafael Verduzco*

2:30 Paper 538h: Development of an Anisotropic Coarse-Grained Conjugated Polymer Model for Optoelectronic Applications — ***Alec S. Bowen***, *Nicholas Jackson, Daniel Reid, Yamil J. Colón, Juan de Pablo*

2:45 Paper 538i: Automated Quantitative Analysis of Oriented Morphologies and Inter-Grain Connectivity in Conjugated Polymers
— ***Nils Persson***, *Michael McBride, Martha A. Grover, Elsa Reichmanis*

(539) Continuous Processing Technologies Applied in Drug Substance Development Crystallization and Drying
Wednesday, Nov 1, 12:30 PM
MCC, 204A/B

Joe Hannon, Chair
Mark Barrett, Co-Chair

Sponsored by:
Pharmaceutical Discovery, Development and Manufacturing Forum

12:30 Paper 539a: Scientific Considerations on Continuous Crystallization and Its PAT Method Validation — ***Xiaochuan Yang***, *David A. Acevedo, Adil Mohammad, Naresh Pavurala, Wei-Lee Wu, Thomas O'Connor, Sau Lee, Patrick J. Faustino, Zoltan K. Nagy, Celia N. Cruz*

12:52 Paper 539b: An Engineering Approach to Concentration of Temperature-Sensitive Pharmaceutical Process Streams for Continuous Crystallization of an API
— ***Phillip Roche***, *Gladys Kate Pascual, Roderick Jones, Philip Donnellan, Brian Glennon*

1:14 Paper 539c: The Effect of Axial Dispersion on Crystal Size Distribution in a Meso-Scale Continuous Oscillatory Baffled Crystallizer — ***Iyke Onyemelukwe***, *Qinglin Su, Zoltan K. Nagy, Chris Rielly*

1:36 Paper 539d: Continuous Heterogeneous Crystallization and the New Method of Making Tablets
— ***Nima Yazdanpanah***, *Allan S. Myerson, Bernhardt L. Trout*

1:58 Paper 539e: A Comparative Study of Continuous Crystallization in an Oscillatory Baffled Crystallizer and a Mixed-Suspension-Mixed-Product-Removal Crystallizer
— ***Claire Yiqing Liu***, *Alastair Barton, Paul Firth, Jonathon Speed, Dan Wood, Zoltan K. Nagy*

2:20 Paper 539f: Continuous Drying of Pharmaceuticals — ***Manuel Kreimer***, *Isabella Aigner, Stephan Sacher, Markus Krumme, Thomas Mannschott, Peter van der Wel, Albert Kaptein, Johannes G. Khinast*

2:42 Paper 539g: Continuous Fluidized Bed Drying of Pharmaceutical Materials
— ***Hao Chen***, *Fernando Muzzio, Benjamin Glasser*

(540) Developments in Extractive Separations: Solvents
Wednesday, Nov 1, 12:30 PM
MCC, M100D

George S. Goff, Chair
Matthaeus Siebenhofer, Co-Chair
Megan E. Donaldson, Co-Chair

Sponsored by: Extractions

12:30 Paper 540a: Thermodynamic Studies and Process Modeling for the Separation of Aromatics from Aliphatics with Ionic Liquids — ***Yuanyuan Lyu***, *Joan F. Brennecke, Mark A. Stadtherr*

12:55 Paper 540b: Equilibrium Data Determination for Sucrose Esters Separation — *Maria F. Gutierrez,* ***Andrea Suaza***, *Jose L. Rivera, Alvaro Orjuela*

1:20 Paper 540c: A Molecular Design Method Based on the COSMO-SAC Model for Ionic Liquid in Extractive Distillation — ***Jing Fang***, *Chunli Li, Yijing Wang, Rui Zhao*

1:45 Paper 540d: Replacement of Toxic Organic Solvents with Natural Non-Toxic Diluents for the Recovery of Pyruvic Acid — ***Mustafa E. Marti***, *Hani Zeidan*

2:10 Paper 540e: Efficient Extraction of Phenolic Compounds from Oils with Dicationic Ionic Liquids via Forming Deep Eutectic Solvents — *Youan Ji, Yucui Hou, Shuhang Ren, Congfei Yao,* ***Weize Wu***

2:35 Paper 540f: Supercritical Extraction of Essential Oil from Achillea wilhelmsii: Experiments and Modelling — ***Bizhan Honarvar***, *Davood Cheraghi Il*

(541) Diagnostics, Treatments and Theranostics
Wednesday, Nov 1, 12:30 PM
MCC, 202A/B

Hedieh Saffari, Chair
Huanan Zhang, Co-Chair

Sponsored by:
Chemical Engineers in Medicine

12:30 Paper 541a: Protein and Gold Nanoparticle-Based Radiation Sensor — ***Amar Thaker***, *Karthik Pushpavanam, Kaushal Rege, Brent L. Nannenga*

12:55 Paper 541b: Direct Detection of Nucleic Acids Without Amplification
— ***Zachary McGee***, *Savannah Dewberry, Carter Wright, Paula Koelle, Peggy Sammon, Krishnan Chittur*

1:20 Paper 541c: Photoacoustic Imaging to Simultaneously Detect the Accumulation of Multiple Contrast Agents Within Tumors
— ***Leon Z. Wang***, *Hoang D. Lu, Tristan Lim, Brian K. Wilson, Andrew Heinmiller, Robert K. Prud'homme*

1:45 Paper 541d: DNA Methylation Detection with an Engineered Protein That Binds Hemi-Methylated DNA
— ***Brooke E. Tam***, *Ki-Joo Sung, Yining Hao, Dana B. Dabbousi, Hadley D. Sikes*

2:10 Paper 541e: Effective Physiological and Anatomical Parameters on Fractional Fluid Reserve (FFR) of Coronary Artery Stenosis
— ***Javad Hashemi***, *R. Eric Berson, Shahab Ghafghazi*

2:35 Paper 541f: Analysis of Carbonyl Compounds in Exhaled Breath for Identification of Lung Cancer Biomarkers — ***Qi Li***, *Mingxiao Li, Michael H. Nantz, Xiao-an Fu*

(542) Drug Delivery II
Wednesday, Nov 1, 12:30 PM
MCC, 208B

Christopher A. Alabi, Chair
Forrest Kievit, Co-Chair

Sponsored by:
Engineering Fundamentals in Life Science

12:30 Paper 542a: Transdermal Protein Delivery via a Choline-Based Deep Eutectic Solvent — ***Kelly Ibsen***, *Amrita Banerjee, Yasunori Iwao, Michael Zakrewsky, Samir Mitragotri*

12:48 Paper 542b: Enhanced Delivery to Skin Using Novel Terbinafine Ionic Liquids — ***Wilmarie Medina-Ramos***, *Mark R. Prausnitz*

1:06 Paper 542c: Controlled Release of N-Acetylcysteine Positively Affects the Viability, Redox State and Morphology of Oligodendrocyte Progenitor Cells Under Oxidative Stress
— ***Nick P. Murphy***, *Kyle Lampe*

1:24 Paper 542d: Gold Nanocones: A Candidate for Cavitation-Enhanced Drug Delivery — *Xiaoqian Su,* ***James J. Kwan***

1:42 Paper 542e: Crossing the Blood-Brain Barrier at the Nanoscale: Understanding the Influence of Physical Characteristics — ***Maksymilian Nowak***, *Tyler D. Brown, Matthew E. Helgeson, Samir Mitragotri*

2:00 Paper 542f: Targeted Drug Delivery to the Back of the Eye by Hydrogel Pushing in the Suprachoroidal Space — ***Jae Hwan Jung***, *Patcharin Desit, Mark R. Prausnitz*

2:18 Paper 542g: Polymerizable Prodrug Monomers for the Treatment of Serious Intracellular Bacterial Infections
— ***Anthony J. Convertine***

(543) Dynamic Processes at Interfaces
Wednesday, Nov 1, 12:30 PM
MCC, M100A

Ilona Kretzschmar, Chair
Siowling Soh, Co-Chair
Jaime Juárez, Co-Chair

Sponsored by: Interfacial Phenomena

12:30 Welcoming Remarks

12:33 Paper 543a: Elevated-Pressure Interfacial Dynamics of LS Surfactants at the Water-CO_2 Interface
— ***Zachary R. Hinton***, *Nicolas J. Alvarez*

12:49 Paper 543b: Atomistic Simulations of Micellization and Adsorption of Imidazoline-Based Surfactants near Metal-Water Interfaces
— ***Sumit Sharma***, *Yathish Kurapati*

1:05 Paper 543c: Surfactant Chemistry and Counter-Ion Clouds in Bile Salt–Stabilized SWCNTs — ***Ketan S. Khare***, *Frederick R. Phelan Jr.*

1:21 Paper 543d: Tailoring Inhibitors of Pathological Crystallization: New Platforms for Drug Design
— ***Bryan Alamani***, *Doyoung Kim, Mangalaa Dinivahi, Diego Guala, Brandon Melendez, Jeffrey D. Rimer*

1:37 Paper 543e: Directed Crystal Nucleation and Growth of Blue Phases by Chemically Patterned Surfaces — ***Xiao Li***, *Jose Martinez-Gonzalez, Juan Hernandez-Ortiz, Ye Zhou, Monirosadat Sadati, Rui Zhang, Juan De Pablo, Paul F. Nealey*

1:53 Paper 543f: Transient Reorientation of Liquid Crystals Induced by Water Transport
— ***Hadi Ramezani-Dakhel***, *Monirosadat Sadati, Rui Zhang, Mohammad Rahimi, Khia Kurtenbach, Nicholas L. Abbott, Benoit Roux, Juan de Pablo*

2:09 Paper 543g: Investigation of Dynamic Surface Tension Induced by Gas-Liquid Absorption in a Microfluidic Device — ***Lu Yang***

2:25 Paper 543h: DNA-Micropost Adsorption and Enhanced Transport in More Crowded Micropost Arrays
— ***Yeng-Long Chen***, *Wei Chien, Fan-Tso Chien*

2:41 Paper 543i: A Miniaturized, Radial Langmuir Trough for Simultaneous Visualization and Dilatational Deformation of a Complex Fluid-Fluid Interface — ***Joseph R. Samaniuk***

2:57 Concluding Remarks

(544) Efficient Processing of Lignin to Bioproducts and Biofuels I
Wednesday, Nov 1, 12:30 PM
MCC, 103B

Bin Yang, Chair
Arthur J. Ragauskas, Co-Chair
Johnway Gao, Co-Chair
Joshua Yuan, Co-Chair

Sponsored by:
Innovations of Green Process Engineering for Sustainable Energy and Environment

12:30 Paper 544a: Structural Characterization and Catalytic Valorization of Co-Solvent Enhanced Lignocellulosic Fractionation Pretreated Lignin — ***Xianzhi Meng***, *Charles M. Cai, Yunqiao Pu, Aakash Parikh, Charles Wyman, Arthur J. Ragauskas*

12:55 Paper 544b: Group IB Metal-Activated Anatase TiO_2 for Selective Catalytic Deoxygenation of Lignin Fragments — *Jingbo Mao, Kairui Liu, Xiaoqiang Zhang, Qi Fang,* ***Z. Conrad Zhang***

1:20 Paper 544c: Recovery of Coumaric and Ferulic Acids from Industrial Lignin Streams
— ***Marjorie Rover***, *Patrick Johnston, Ryan Smith, Robert C. Brown*

1:45 Paper 544d: Enabling Bioconversion of Biorefinery Wastes to Lipids with Oleaginous *Rhodococci*
— *Xiaolu Li, Zhangyang Xu, Yucai He,* ***Bin Yang***

2:10 Paper 544e: Understanding Trends in Hydrodeoxygenation of Biomass-Derived Phenolics from C-C Versus C-O Scission Reaction in Ethanol on Stepped Surfaces
— ***Fatima Jalid***, *Tuhin Suvra Khan, M. Ali Haider*

2:35 Paper 544f: Lignin Conversion and Upgrading to High–Octane Number Gasoline — ***Maoqi Feng***, *Bin Yang*

(545) Emerging Applications of Cellulose Nanofibrils (CNFs) and Its Composites
Wednesday, Nov 1, 12:30 PM
MCC, 200B

Sudhagar Mani, Chair
Joseph F. Stanzione III, Co-Chair

Sponsored by:
Forest and Plant Bioproducts Division

12:30 Paper 545a: Spray-Coating Chitin & Cellulose Nanomaterials for Enhancement of Barrier Properties
— ***Chinmay C. Satam***, *Jerel Jallorina, J. Carson Meredith*

12:55 Paper 545b: Development of Low-Concentration Alkaline Treatment Method to Produce Thermally Stable Cellulose Nanofibrils (CNFs)
— ***Hansol Lee***

1:20 Paper 545c: Tailored and Integrated Production of Carboxylated and Lignin-Containing Cellulose Nanocrystals and Nanofibrils for Composite Applications — ***J. Y. Zhu***

1:45 Paper 545d: Nano Carbon Structures from Cellulosic Biomass for Use as Functional Materials
— ***Ping Wang***

(546) Energetic and Reactive Materials
Wednesday, Nov 1, 12:30 PM
MCC, 200J

Travis R. Sippel, Chair
Lori J. Groven, Co-Chair

Sponsored by: Energetics

12:30 Paper 546a: The Use of Genetic Algorithms to Predict the Crystal Structures of Energetics
— ***Clinton Chapman***, *Kevin Hadley*

12:45 Paper 546b: Investigation of Ignition in HMX Using the Henson-Smilowitz Reaction Model
— ***Sushilkumar Koundinyan***, *Nirmal Rai, H. S. Udaykumar*

1:00 Paper 546c: Combustion Studies of Microscale Aluminum Functionalized with Perfluorotetradecanoic Acid
— ***Loudon Campbell***, *Dylan Smith, Kevin Hill, Michelle Pantoya, Rebecca Wilson*

1:15 Paper 546d: Fuel-Rich Metallic Energetics with Metal-Fluoride Oxidizers — ***Siva Kumar Valluri***, *Ian Monk, Mirko Schoenitz, Edward L. Dreizin*

1:30 Break

1:35 Paper 546e: Nanocomposite Thermite Powders with Improved Flowability Prepared by Mechanical Milling — ***Quang Nguyen***, *Ci Huang, Mirko Schoenitz, Kyle Sullivan, Edward Dreizin*

1:50 Paper 546f: Doping Boron with Iron for Better Combustion
— ***Kerri-Lee A. Chintersingh***, *Mirko Schoenitz, Edward L. Dreizin*

2:05 Paper 546g: Synthesis and Reactive Characterization of Aluminum Combined with Aluminum Iodate Hexahydrate Crystals $[Al(H_2O)_6](IO_3)_3(HIO3)_2$ — ***Dylan Smith***, *Daniel Unruh, Michelle Pantoya*

2:20 Paper 546h: Magnesium Diboride as a Fuel for Biocidal Formulations
— ***Hannah Dudak***

2:35 Paper 546i: Fused Deposition Modeling of Biocidal Formulations
— ***Lori J. Groven***

(547) Energy System Design I
Wednesday, Nov 1, 12:30 PM
MCC, 103C

Joseph Scott, Chair
Dharik Mallapragada, Co-Chair
Donald J. Chmielewski, Co-Chair

Sponsored by:
Systems and Process Design

12:30 Paper 547a: Go Now or Wait and See? Optimal Investment Timing in National Power Systems
— ***Clara F. Heuberger***, *Iain Staffell, Nilay Shah, Niall Mac Dowell*

12:51 Paper 547b: Beyond LCOE: Market-Based Design of Flexible Solar Thermal Systems — ***Alexander W. Dowling***, *Tian Zheng, Xinyue Peng, Christos Maravelias, Thatcher W. Root, Victor M. Zavala*

1:12 Paper 547c: Enterprise-Wide Modular Process Intensification and Multiscale Optimization for Natural Gas Utilization — ***Shachit S. Iyer***, *Salih E. Demirel, M. M. Faruque Hasan*

1:33 Paper 547d: Development of a Superstructure for Work and Heat Exchange Networks (WHENs) — ***Matias Vikse***, *Chao Fu, Paul I. Barton, Truls Gundersen*

1:54 Paper 547e: Multiresolution Modeling and Optimization of a Natural Gas Liquefaction Process Using Detailed Spiral-Wound Heat-Exchanger Models — ***Calvin Tsay***, *Richard Pattison, Michael Baldea*

2:15 Paper 547f: Optimal Design and Dynamic Modeling of Microtube Recuperators in an Indirect Supercritical Carbon Dioxide Recompression Brayton Power Cycle — ***Yuan Jiang***, *Eric A. Liese, Stephen E. Zitney, Debangsu Bhattacharyya*

2:36 Paper 547g: Locating Heat Exchangers in an EIP-Wide Heat Integration Network — ***Sajitha K. Nair***, *Melvin Soon, Iftekhar A. Karimi*

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(548) Environmental Advances in Nuclear and Hazardous Waste Treatment II

Wednesday, Nov 1, 12:30 PM
MCC, 102E

Robert W. Peters, Chair
Thong Hang, Co-Chair
Ramesh Chawla, Co-Chair
Eunsung Kan, Co-Chair

Sponsored by:
Solid and Hazardous Waste

12:30 Paper 548a: Prediction of Cesium Loading on Crystalline Silicotitanate Ion-Exchange Resin — ***Thong Hang***, *L. Larry Hamm, Daniel J. McCabe, Jennifer L. Wohlwend*

1:00 Paper 548b: Computational Optimization of Difficult Physics-Based Project Designs Using Massively Parallel Solution Methods — ***Larry M. Deschaine***

1:30 Paper 548c: An Evaluation of Organically Bound Tritium (OBT) Research — ***Sandra Cutts***, *Robin L. Brigmon, John Seaman, Robert W. Peters*

2:00 Paper 548d: 3D-Interconnected PVA-Citric Acid Porous Hydrogels Embedded with Potassium-Copper Hexacyanoferrate Nanoparticles for Enhanced Removal of Radionuclide Cesium — ***Yun Kon Kim***, *Yonghwan Kim, Sungjun Kim, David Harbottle, Jae W. Lee*

(549) Environmental Applications of Nanotechnology and Nanomaterials II

Wednesday, Nov 1, 12:30 PM
MCC, 210A/B

Larry Erickson, Chair
Placidus B. Amama, Co-Chair
Tapas K. Das, Co-Chair

Sponsored by:
Environmental Aspects, Applications, and Implications of Nanomaterials and Nanotechnology

12:30 Paper 549a: Procyanidin-Assisted Synthesis of Fe-Pd Nanoparticles for Superior Dechlorination of p-Chlorophenol — ***Mingyue Liu***, *Rongxin Su, Wei Qi, Zhimin He*

12:55 Paper 549b: Synthesis of Ni/γ-Al_2O_3 Catalysts for Methanation of CO_2 at Low Temperature Under Atmospheric Pressure — ***Waqar Ahmad***, ***Reyad Shawabkeh***, ***Shakeel Ahmed***

1:20 Paper 549c: Development of Multifaceted AgNPs with the Aid of Green Chemistry for Synergistic Combating Effect on Phytopathogens, Catalytic Efficiency on Anthropogenic Pollutants and Free-Radical Scavenging Activity — ***Arulmozhi M***, *Jayapriya M, Balraj B.*

1:45 Paper 549d: Applications of Heterogeneous Fenton Catalysts in Pollutant Degradation, Sensing, and Cancer Treatments — ***Shih-Yuan Lu***

2:10 Paper 549e: Application of Entrapped Nano-Zero-Valent Iron into Cellulose Acetate Membranes for Domestic Wastewater Treatment — ***Mohamed K. Mostafa***, *Ahmed S. Mahmoud, Rasha A. SaryEl-deen, Robert W. Peters*

2:35 Paper 549f: The Role of Carbon Nanotubes in Photocatalytic Conversion of CO_2/H_2O and CO_2/CH_4 Systems to Syngas — ***Karishma Piler***, *Paul Bernazzani, Tracy J. Benson, Cristian Bahrim*

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(550) Experimental, Theoretical, and Numerical Analysis of Transport Processes in Flow Reactors

Wednesday, Nov 1, 12:30 PM
MCC, 200F

Cory Jensen, Chair
Ravindra Aglave, Co-Chair

Sponsored by:
Transport and Energy Processes

12:30 Paper 550a: Methanol Partial Oxidation on Silver in a Fixed Bed of Raschig Rings: An Integrated CFD with Microkinetics Study — ***Behnam Partopour***, *Anthony G. Dixon*

12:52 Paper 550b: Application of Recent Understanding of Intra-Molecular Forces and Micro-Hydrodynamics to the Bubble Dynamics and Gas-Liquid Transfer in a Downward-Flow Microbubble Column — ***Manizheh Ansari***, *Damon Turney, Sanjoy Banerjee, J. B. Joshi*

1:14 Paper 550c: A Hybrid Solution for a Heat Transfer Model to Distributed Parameters in the Solid Phase of a Biomass Pyrolysis Reactor — *Juscelino Almeida Junior, Jaci Carlo Schramm Camara Bastos,* ***Vinicyus R. Wiggers***, *Carolina Krebs de Souza, Fernanda Raquel Wust Schmitz, Savio L. Bertoli*

1:36 Paper 550d: Experimental and CFD Simulation Study of Bubble Column Equipped with a Bundle of Heat-Exchanging Tubes (Internals) for Fischer-Tropsch (FT) Synthesis — ***Abbas Sultan***, *Laith Sabri, Hayder Al-Naseri, Muthanna Al Dahhan*

1:58 Paper 550e: Numerical Study of Hydrogen Production via High-Temperature and Low-Temperature Water-Gas Shift Reactors' System: The Multiscale (Pellet-Reactor Scale) Modeling Approach and Simulation — ***Secgin Karagoz***, ***Flavio da Cruz***, *Vasilios Manousiouthakis*

2:20 Paper 550f: A Generalized Semi-Analytical Method for Solution of Ordinary Differential Equations Applied to a Model of Heat Transfer in a Biomass Pyrolysis Reactor — *Juscelino Almeida Junior, Jaci Carlo Schramm Camara Bastos,* ***Laércio Ender***, *Lisiane Fernandes de Carvalho, Licodiedoff Silvana, Savio L. Bertoli*

2:42 Paper 550g: A Numerical Model of Ambient Air Vaporizer and Its Validation with Pilot-Scale Data — ***Yongkyu Lee***, *Jongmin Park, Chonghun Han, Wonbo Lee*

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(551) Forum Plenary: Computational Molecular Science and Engineering Forum (Invited Talks)

Wednesday, Nov 1, 12:30 PM
MCC, L100H

Jeffrey R. Errington, Chair
Coray M. Colina, Co-Chair

Sponsored by:
Computational Molecular Science and Engineering Forum

12:30 Paper 551a: Systematic Multiscale Models and Physics Using the Relative Entropy — ***M. Scott Shell***

1:10 Paper 551b: Development of a Top-Down Coarse-Grained Model for Protein Assemblies — ***Jeetain Mittal***

1:30 Paper 551c: Accessing the Inaccessible: Studying the Liquid-to-Solid Transition in Molecular Simulations — ***Sapna Sarupria***

1:50 Paper 551d: A Brief History of Exploring Hypothetical Crystal Structures — ***Christopher E. Wilmer***

2:30 Paper 551e: Molecular Modeling of Adsorption of CO_2 and Water in Hydrophobic Metal-Organic Frameworks — ***Randall Q. Snurr***, *Peyman Z. Moghadam, Hongda Zhang*

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(552) Free Forum on Engineering Education: First Year and Sophomore Year

Wednesday, Nov 1, 12:30 PM
MCC, 205D

Jeffrey Rice, Co-Chair
Gerold A. Willing, Co-Chair
Jason White, Co-Chair

Sponsored by:
Undergraduate Education

12:30 Paper 552a: Measuring Impacts of Course Changes in Introduction to Chemical Engineering — ***Joshua A. Enszer***, *Arthi Jayaraman*

12:50 Paper 552b: Seeing Is Learning: Showing First-Year Undergraduate Students a Preview of Senior-Level Chemical Engineering Experiments — ***Aravind Suresh***

1:10 Paper 552c: Visualization of Newtonian Pipe Flow Around Static Mixers: 3-D Printing Applications in the ChE Curriculum — ***Connor Gavin***, *Alexander R. Ivans, Max E. Serraty, Zenaida Otero Gephardt*

1:30 Paper 552d: An Introduction to Design for Chemical Engineering Undergraduates — ***Daryl Williams***

1:50 Paper 552e: The Engineering and Computing Residential Living and Learning Community at the University of South Carolina — ***Edward P. Gatzke***, *Jed Lyons, Ruth Patterson, Nigel Word*

2:10 Paper 552f: Progressive Development of Students' Capacities to Engage in Functional Teaming — ***Natasha Mallette***, *Michelle Bothwell,* ***Milo D. Koretsky***

2:30 Paper 552g: The Use of Numerical Worksheets for Material and Energy Balances Course — ***Satish J. Parulekar***

(553) Fuel Processing for Hydrogen Production

Wednesday, Nov 1, 12:30 PM
MCC, 200C

Dushyant Shekhawat, Chair
David Berry, Co-Chair
Daniel J. Haynes, Co-Chair
Scott McWhorter, Co-Chair

Sponsored by:
Advances in Fossil Energy R&D

12:30 Paper 553a: Reforming of Hydrocarbons for Hydrogen Generation: HyRes — ***Girish Srinivas***, *Staci A. Van Norman, Steven Gebhard, Steven Schwab*

12:49 Paper 553b: Syngas Production on Thermally Conductive SiC Catalyst — ***Seungdoo Park***, *Naftali Opembe, Sergio Ibanez, Doug Mitchell, Matthew Seabaugh, Scott Swartz*

1:08 Paper 553c: Preliminary Studies on Catalytic Open Cells Foams Methane Combustion Recovered from Fuel Processor Systems — ***Giuliana Ercolino***, *Carmen Williana Moncada Quintero, Stefania Specchia*

1:27 Paper 553d: Thermodynamic Simulations, Experiments and Techno-Economic Analysis of Iron-Based Chemical-Looping Systems for H_2 Production — ***Mandar Kathe***, *Liang-Shih Fan, Frank Kong*

1:46 Paper 553e: Development of Thermo-Neutral Reforming Catalyst for On-Board Hydrogen Production — ***Shakeel Ahmed***, *Fahad Al-Muhaish, Uwais Baduruthamal, Sai P. Katikaneni, Aadesh X. Harale*

2:05 Paper 553f: 1 kW_e Diesel Autothermal Reformer Integrated with Catalytic Burner for Exhaust Gas Oxidation — ***Minseok Bae***, ***Jiwoo Oh***, *Hyungjun Jeon, Dongyeon Kim, Joongmyeon Bae, Sai P. Katikaneni*

2:24 Paper 553g: CFD Study of a Pilot-Scale Multi-Tube Palladium Membrane Module for Hydrogen Separation— ***Rui Ma***, *Bernardo Castro Dominguez, Ivan Mardilovich, Nikolaos Kazantzis, Anthony G. Dixon, Yi Hua Ma*

2:43 Paper 553h: Novel SAPO-34 Hollow Fiber Membrane for H2 Separation Under Various Gas Atmospheres at High Temperature — ***Zhigang Wang***, *Nikita Dewangan, Sonali Das, Sibudjing Kawi*

(554) Fundamentals of Electrode Processes II

Wednesday, Nov 1, 12:30 PM
MCC, M100C

Elizabeth J. Biddinger, Co-Chair
Christopher G. Arges, Co-Chair

Sponsored by:
Electrochemical Fundamentals

12:30 Paper 554a: Electrocatalytic CO_2 Reduction for Enhanced C-C Coupling — ***Youngkook Kwon***

12:50 Paper 554b: Advances in Mesoscale Modeling of Lithium-Ion Battery Cathodes — ***Scott A. Roberts***, *Bradley L. Trembacki, Mark E. Ferraro*

1:10 Paper 554c: Reaction Path Discovery Under Potential Bias — ***Eric Walker***, *Paul M. Zimmerman*

1:30 Break

2:00 Paper 554e: Electrocatalytic Carbon Fixation on Molecular-Material Hybrids — ***Zhi Cao***, *Christopher Chang*

2:20 Paper 554f: Investigation of the Morphological Factors That Drive Selectivity on Polycrystalline Cu During CO_2 Electroreduction — *Alexandros N. Karaiskakis,* ***Elizabeth J. Biddinger***

2:40 Paper 554g: Modulation of Charge Transfer Kinetics by Two Orders of Magnitude at Back-Gated Monolayer MoS_2 Electrodes — ***Yan Wang***, *C. Daniel Frisbie*

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(555) Fundamentals of Oxide Catalysis

Wednesday, Nov 1, 12:30 PM
MCC, L100F

Taejin Kim, Chair
Prashant Deshlahra, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

12:30 Paper 555a: Fundamental Investigation of C-C Coupling of Carbonyl Compounds on Ceria — ***Chuanlin Zhao***, *Aditya Savara, Ye Xu*

12:50 Paper 555b: N_2O Dissociation on Co_3O_4-Based Catalysts: Reducibility of Co_3O_4 and Its Catalytic Consequences — ***Yongchun Hong***, *Andrew (Bean) Getsoian, Christine Lambert, Enrique Iglesia*

1:10 Paper 555c: The Effect of Support Morphology on Co/CeO_2 Catalysts for the Reduction of NO by CO — ***Louisa Savereide***, *Justin M. Notestein*

1:30 Paper 555d: Computational Study of Selective Oxidation of Ethane on Oligomeric VO_x/SiO_2 and Bulk Mixed-Oxide Catalysts — ***Yilang Liu***, *Prashant Deshlahra*

1:50 Paper 555e: Computationally Enhanced Spectroscopic Studies of Supported Vanadium Oxide — ***Nicholas Jaegers***, *Chuan Wan, Mary Hu, Monica Vasiliu, David A. Dixon, Eric D. Walter, Israel E. Wachs, Yong Wang, Jian Z. Hu*

2:10 Paper 555f: Mechanistic Origins of Unselective Products in Acrolein Synthesis on Mixed Metal Oxide Catalysts — ***Linh Bui***, *Aditya Bhan*

2:30 Paper 555g: Silica as a Redox Support for Enhanced CO_2 to CO by Perovskite Oxides in the Reverse Water-Gas Shift Chemical-Looping Process — ***Bryan J. Hare***, *Debtanu Maiti, Yolanda A. Daza, Venkat R. Bhethanabotla, John Kuhn*

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(556) Fundamentals of Thermal Deconstruction

Wednesday, Nov 1, 12:30 PM
MCC, 101I

Gregg T. Beckham, Chair

Sponsored by:
Thermal Deconstruction of Biomass

12:30 Paper 556a: Molecular Modeling of Pyrolysis — ***Phillip R. Westmoreland***

12:55 Paper 556b: Kinetics and Energetics of Biomass Pyrolysis by Pulse-Heated Analysis of Solid Reactions (PHASR) — ***Paul J. Dauenhauer***

1:20 Paper 556c: Theoretical Elucidation of the Molecular Behaviours of Key Compounds During Biomass Pyrolysis — ***Xiaolei Zhang***

1:45 Paper 556d: Study of Red Oak-Derived Lignin, Pyrolytic Lignin, and Hydrogenated Pyrolytic Lignin with 2D-NMR, FTICR-MS, and GPC — *Daniel J. McClelland, Ali Hussain Motagamwala, Marjorie R. Rover, Ashley Wittrig, Chunping Wu, John Ralph, Robert Brown, James Dumesic,* ***George W. Huber***

2:10 Paper 556e: Overview of Issues Around Deconstruction of Lignin — ***Marcus Foston***

2:35 Paper 556f: Mesoscale Modeling of Thermochemical Conversion of Biomass — ***Peter N. Ciesielski***, *Brennan Pecha*

(557) Graphene and Carbon Nanotubes: Characterization, Functionalization, and Dispersion

Wednesday, Nov 1, 12:30 PM
MCC, 213A/B

Carlos A. Silvera Batista, Chair
Vida Jamali, Co-Chair
Megan A. Creighton, Co-Chair

Sponsored by: Carbon Nanomaterials

12:30 Paper 557a: Environmental Effects on DNA Binding to Single-Wall Carbon Nanotubes — ***Niyousha Mohammadshafie***, *Geyou Ao*

12:55 Paper 557b: Modifying Single-Wall Carbon Nanotubes Properties Through Endohedral Filling — ***Jeffrey A. Fagan***

1:20 Paper 557c: Retained Carrier-Mobility and Enhanced Plasmonic-Photovoltaics of Graphene via Ring-Centered η^6 Functionalization and Nano-Interfacing — *Songwei Che, Kabeer Jasuja, Sanjay Behura, Phong Nguyen, Sreenivasan Sreeprasad,* ***Vikas Berry***

1:45 Paper 557d: Preparation of Polyacrylonitrile and Polyacrylonitrile/Carbon Nanostructures — ***Vahid Alizadeh***

2:10 Paper 201aj: Sustainable Design of Carbon Nanomaterials: Decoupling the Role of Material Structure and Surface Chemistry on Electrochemical and Biological Activities — *Yan Wang,* ***Leanne Gilbertson***

2:35 Paper 557f: Mechanical Behavior of Nanocomposite Structures from Interlayer Bonding in Twisted Bilayer Graphene — ***Mengxi Chen***, *Andre R. Muniz, Dimitrios Maroudas*

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(558) Modeling and Computation in Energy and Environment

Wednesday, Nov 1, 12:30 PM
MCC, 103F

Masoud Soroush, Chair
Yash Puranik, Co-Chair

Sponsored by:
Applied Mathematics and Numerical Analysis

12:30 Paper 558a: Thermochemical and Catalytic-Upgrading System Design to Convert Biomass to Liquid Fuel Using a Superstructure-Based Approach — ***Gautham Madenoor Ramapriya***, *Wangyun Won, Christos T. Maravelias*

TECHNICAL SESSIONS 2017

An up-to-date program is available at www.aiche.org/annual or on the Annual Meeting app
Please refrain from photographing slides or taking video of sessions and presentations.

12:49 Paper 558b: Kepler Workflow in a Cloud Infrastructure for Temperature Balancing in a Steam Methane Reformer Furnace Using a Computational Fluid Dynamics and a Data-Driven Optimization Approach — ***Andres Aguirre***, *Anh Tran, Yangyao Ding, Prakashan Korambath, Panagiotis D. Christofides*

1:08 Paper 558c: A Multiparametric C.F.D. Analysis of Multiphase Annular Flows for Oil and Gas Drilling Applications — *Emmanuel Epelle,* ***Dimitrios I. Gerogiorgis***

1:27 Paper 558d: Development of a 3D Computational Fluid Dynamics Model for Microbial Fuel Cells — ***Xianhua Li***, *Robert Ferrari, Jaclyn Guglielmi, Zuyi (Jacky) Huang*

1:46 Paper 558e: Optimal Resource Expansion and Placement in Smart Grid Communications Networks — ***Todd Zhen***, *Tarek Elgindy, S. M. Shafiul Alam, Anthony Florita, Bri-Mathias S. Hodge, Carl Laird*

2:05 Paper 558f: Quantification of Parameter Space Regions Consistent with System Models and Associated Experimental Data — ***Jeremy A. Conner***, *Jack Lowd, Richard J. Ciora, Theo Tstosis, Vasilios Manousiouthakis*

2:24 Paper 558g: Design and Intensification of Integrated Carbon Capture and Conversion to Chemicals — ***Shachit S. Iyer***, *Ishan Bajaj, Priyadarshini Balasubramanian, M. M. Faruque Hasan*

2:43 Paper 558h: Response Surface Models for Set Point Determination of Smokeless Steam and Air-Assisted Flares — ***Arokiaraj Alphones***, *Daniel Chen, Helen Lou, Vijaya Damodara, Xianchang Li, Christopher B. Martin, Edward Fortner, Scott Evans, Matthew Johnson*

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(559) Nanobiotechnology for Sensors and Imaging I
Wednesday, Nov 1, 12:30 PM
MCC, 212A/B

Venkat R. Bhethanabotla, Chair
Subramanian Sankaranarayanan, Co-Chair
Daniel Roxbury, Co-Chair

Sponsored by: Bionanotechnology

12:30 Paper 559a: Chirality-Resolved Optical Spectroscopy for Recognition Sequence Identification and Sensor Construction in DNA-Carbon Nanotube Hybrids — *Prakrit Jena, Mohammad Safaee, Daniel Heller,* ***Daniel Roxbury***

12:48 Paper 559b: Antibody-Mimetic Protein Detection with Peptoid-Functionalized Near-Infrared Carbon Nanotube Optical Sensors — ***Linda Chio***, *Jackson Travis Del Bonis-O'Donnell, Mark Kline, Ronald N. Zuckermann, Markita Landry*

1:06 Paper 559c: Measuring Hydrolytic Enzyme Activity with Substrate-Wrapped Single-Walled Carbon Nanotubes for Optimization of Biomass Conversion — ***Nathaniel Kallmyer***, *Nigel Reuel*

1:24 Paper 559d: Photon Upconversion and High-Throughput Optical DNA Sequencing: Putting a Squeeze on Light — ***Prashant Nagpal***

1:42 Paper 559e: Molecular Recognition of Dopamine with Near-Infrared Dual Excitation-Emission Two-Photon Microscopy of Nanosensors — ***Jackson Travis Del Bonis-O'Donnell***, *Ralph Page, Abraham Beyene, Eric Tindall, Ian McFarlane, Markita Landry*

2:00 Paper 559f: Interaction of Single-Walled Carbon Nanotubes (SWCNTs) with Photosynthetic Organisms — ***Alessandra Antonucci***, *Nils Schuergers, Vitalijs Zubkovs, Ardemis A. Boghossian*

2:18 Paper 559g: Fluorescent Single-Wall Carbon Nanotube Microarray for Label-Free, Real-Time Biomolecular Detection and Binding Kinetic Analysis — ***Juyao Dong***, *Michael Strano*

2:36 Paper 559h: Carbon Nanotube Photoluminescence for In-Vivo Biosensors — ***Daniel Heller***, *Jackson Harvey, Prakrit Jena, Thomas Galassi, Ryan Williams, Gül H. Zerze, Jeetain Mittal, Daniel Roxbury*

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(560) NH_3 Fuel End Use
Wednesday, Nov 1, 12:30 PM
MCC, 101F/G

Sponsored by:
NH_3 Energy$^+$ — Enabling Optimized, Sustainable Energy and Agriculture

12:30 Paper 560a: Combustion Emissions from NH_3 Fuel Gas Turbine Power Generation Demonstrated — ***Osamu Kurata***, *Norihiko Iki, Takahiro Inoue, Takayuki Matsunuma, Taku Tsujimura, Hirohide Furutani, Hideaki Kobayashi, Akihiro Hayakawa*

12:48 Paper 560b: Detailed Observation of Coal-Ammonia Co-Combustion Processes — ***Noriaki Nakatsuka***, *Junpei Fukui, Kazuki Tainaka, Hidetaka Higashino, Jun Hayashi, Fumiteru Akamatsu*

1:06 Paper 560c: Development of Materials and Systems for Ammonia-Fueled Solid Oxide Fuel Cells — ***Koichi Eguchi***, *Yosuke Takahashi, Hayahide Yamasaki, Hidehito Kubo, Akihiro Okabe, Takenori Isomura, Takahiro Matsuo*

1:24 Paper 560d: Development of New Combustion Strategy for Internal Combustion Engine Fueled by Pure Ammonia — ***Donggeun Lee***, *Hyungeun Min, Hyunho Park, Han Ho Song*

1:42 Paper 560e: Direct Ammonia Fuel Cell Utilizing an OH- Ion-Conducting Membrane Electrolyte — *Yushan Yan,* ***Shimshon Gottesfeld***

2:00 Paper 560f: Effect of Water on the Auto-Ignition of a Non-Carbon Nitrogen-Based Monofuel — ***Bar Mosevitzky***, *Rotem Azoulay, Lilach Naamat, Gennady E. Shter, Gideon S. Grader*

2:18 Paper 560g: Effects of the Thickness of the Burner Rim, the Velocities of Fuel and Air on Extinction Limit of Ammonia Coaxial Jet Diffusion Flame — Yohei Ishikawa, ***Jun Hayashi***, Hiroyuki Takeishi, Takahiro Okanami, Kimio Iino, Yasuyuki Yamamoto, Yoshiyuki Hagiwara, Fumiteru Akamatsu

2:36 Paper 560h: Efficient and Clean Combustion of Ammonia-Hydrogen -Air Mixtures — ***Hadi Nozari***, ***Arif Karabeyoglu***

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(561) Novel Nanoparticles and Nano-structured Materials for Catalysis — Influence of the Support
Wednesday, Nov 1, 12:30 PM
MCC, 200H

Shu Hu, Chair
Yu Lei, Co-Chair

Sponsored by: Nanoparticles

12:30 Paper 561a: Metal-Organic Frameworks–Encapsulated Metal Nanoparticles for Heterogeneous Catalysis — *Kui Shen,* ***Yingwei Li***

12:50 Paper 561b: Computational Study of an MOF-Supported Single-Site Ni Catalyst for Ethylene Dimerization — ***Jingyun Ye***, *Aaron League, Donald G. Truhlar, Christopher Cramer, Laura Gagliardi, Varinia Bernales, Omar K. Farha, Joseph T. Hupp, Zhanyong Li, Ana E. Platero Prats, Karena Chapman, Donald M. Camaioni, John L. Fulton, Johannes A. Lercher*

1:10 Paper 561c: Two-Dimensional Nanomaterials as Supports for Heterogeneous Catalysis — ***Zhe Li***, *Yanran Cui, Zhenwei Wu, Jeffrey Miller, Fabio H. Ribeiro, Yue Wu*

1:30 Paper 561d: Mitigating the Oxidative Deactivation on a Multi-Faceted Fe Catalyst: A Multiscale Model from First Principles — ***Jacob Bray***, *Alyssa Hensley, Greg Collinge, Yong Wang, Fanglin Che, Jean-Sabin McEwen*

1:50 Paper 561e: Heterogeneous Dephosphorylation Using Ceria Nanocatalysts: Identifying the Active Site and the Rate-Determining Step — ***Michael J. Manto***, *Pengfei Xie, Chao Wang*

2:10 Paper 561f: Surface Reconstruction of Pd Concave Icosahedra: Atomic-Scale Mechanisms from First Principles and Experiments — ***Ahmed Elnabawy***, *Luke Roling, Kyle D. Gilroy, Tung-Han Yang, Jane Howe, Younan Xia, Manos Mavrikakis*

2:30 Paper 561g: Enhanced Catalysis by Optical Nanoantenna Reduced on Monolayer Transition Metal Dichalcogenide — ***D. Keith Roper***, *Jeremy Dunklin, Gregory T. Forcherio, Alexander O'Brien*

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(562) Novel Polymeric Membranes — GS II
Wednesday, Nov 1, 12:30 PM
MCC, M100I

Zachary P. Smith, Co-Chair
Xueyi Zhang, Co-Chair
Bhupendar Minhas, Co-Chair

Sponsored by:
Membrane-Based Separations

12:30 Paper 562a: A Comprehensive Analysis of Gas Sorption and Transport in Thermally Rearranged Polymers — ***Michele Galizia***, *Kevin A. Stevens, Zachary Smith, Donald R. Paul, Benny D. Freeman*

12:48 Paper 562b: Ionic Polyimides: New Dimensions in the Design of Polymer Gas Separation Membranes — ***Jason E. Bara***, *Grayson P. Dennis, Brian Flowers, Kathryn O'Harra*

1:06 Paper 562c: Tailoring Backbone Rigidity of Triptycene-Containing Polymers for Enhanced Gas Transport Properties — ***Ruilan Guo***, *Jennifer Weidman, Shuangjiang Luo*

1:24 Paper 562d: Ultrathin and Pinhole-Free Gas-Selective Polymeric Films Synthesized via Chemical Vapor Deposition — ***Minghui Wang***, *Nicolas Boscher, Katja Heinze, Alberto Perrotta, Mariadriana Creatore, Karen K. Gleason*

1:42 Paper 562e: The Effects of Backbone Chemical Structure on Gas Transport Properties in a Family of Polyethersulfones Polymers — ***Ali Naderi***, *Yong Wai Fen, Youchang Xiao, Neal Chung, Martin Weber, Christian Maletzko*

2:00 Paper 562f: Hydrophilic and Morphological Modification of Polyethersulfone Substrates for Composite Membranes in CO_2 Separation — ***Dongzhu Wu***, *Yang Han, Witopo Salim, Kai Chen, W. S. Winston Ho*

2:18 Paper 562g: Comparison Between Perfluoropolymers and Hydrocarbon Polymer Analogs with Pendant Rings for Membrane Gas Separation — ***Milad Yavari***, *Minfeng Fang, Yoshi Okamoto, Haiqing Lin*

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(563) NSF Workshop I: Highlights from CBET
Wednesday, Nov 1, 12:30 PM
MCC, 101H

William L. Olbricht, Chair
Ram B. Gupta, Co-Chair

Sponsored by: Graduate Education

12:30 Paper 563a: Overview of Chemical, Bioengineering, Environmental, and Transport Systems Division (CBET) — *JoAnn S. Lighty*

12:55 Paper 563b: Highlights of CBET Cluster on Chemical and Biochemical Systems — ***Carole Read***

1:15 Paper 563c: Highlights of CBET Cluster on Engineering Biology and Health — ***Steven Peretti***

1:35 Paper 563d: Highlights on CBET Cluster on Environmental Engineering and Sustainability — ***Bruce Hamilton***

1:55 Paper 563e: Highlights of CBET Cluster on Transport, Thermal and Fluid Phenomena — ***William L. Olbricht***

2:15 Paper 563f: Interactive Question and Answer Session with NSF Program Directors — ***Carole Read***, *Steven Peretti, Bruce Hamilton, Robert W. McCabe, T. J. Mountziaris*

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(564) Optimization and Predictive Control
Wednesday, Nov 1, 12:30 PM
MCC, 103D

Jin Wang, Chair
Debangsu Bhattacharyya, Co-Chair

Sponsored by:
Systems and Process Control

12:30 Paper 564a: NMPC of Semi-Batch Processes Under Uncertainty Using Pontryagin's Minimum Principle — ***Erdal Aydin***, *Dominique Bonvin, Kai Sundmacher*

12:49 Paper 564b: Sample-Free Stochastic Nonlinear Model Predictive Control — ***Joel Paulson***, *Vinay Bavdekar, Ali Mesbah*

1:08 Paper 564c: Real-Time Optimization via Modifier Adaptation: On Updating the Model Outputs — *Aris Papasavvas, Tafarel de Avila Ferreira, Alejandro Marchetti,* ***Dominique Bonvin***

1:27 Paper 564d: Nonlinear Model Predictive Control for Zone Tracking — ***Su Liu***, *Jinfeng Liu*

1:46 Paper 564e: Fast, Robust Nonlinear Model Predictive Control Based on Sensitivity Update — ***Zhou (Joyce) Yu***, *Lorenz T. Biegler, Thomas A. Badgwell*

2:05 Paper 564f: Fault-Tolerant Economic Model Predictive Control with Empirical Process Models — *Anas Alanqar,* ***Helen Durand***, *Panagiotis D. Christofides*

2:24 Paper 564g: Fault-Tolerant Model Predictive Control of Nonlinear Process Systems Using a Forecast-Triggered Communication Strategy — ***Da Xue***, *Nael H. El-Farra*

2:43 Paper 564h: Multi-Grid Schemes for Multiscale Predictive Control — ***Sungho Shin***, *Victor M. Zavala*

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(565) PAT for Process Understanding, Reduced Testing, and Elucidation of Fundamental Phenomena in Drug Product/ Substance Development
Wednesday, Nov 1, 12:30 PM
MCC, 201A/B

Nima Yazdanpanah, Chair
Shujauddin M. Changi, Co-Chair

Sponsored by:
Pharmaceutical Discovery, Development and Manufacturing Forum

12:30 Introductory Remarks

12:35 Paper 565a: Residence Time Distribution and Segregation Studies Through Real-Time Measurements by Near-Infrared Spectroscopy — ***Andrés D. Román-Ospino***, *Sarang Oka, Sara Moghtadernejad, M. Sebastian Escotet-Espinoza, Ravendra Singh, Rohit Ramachandran, Marianthi Ierapetritou, Fernando Muzzio*

12:55 Paper 565b: Use of Process Analytical Technology (PAT) in Advanced Manufacturing Process Monitoring and Control: Scientific Considerations and Regulatory Challenges — ***Huiquan Wu***

1:15 Paper 565c: 3D Raman Imaging: A Method to Study the Effects of Lubrication on the Microstructure of Tablets — ***Shashwat Gupta***, *Savitha Panikar, Fernando J. Muzzio*

1:35 Paper 565d: Development and Validation of an In-Line NIR Spectroscopic Method for Continuous Blend Potency Determination in the Feed Frame of a Tablet Press — ***Fien De Leersnyder***, *Elisabeth Peeters, Djalabi Hasna, Valérie Vanhoorne, Bernd Van Snick, Ke Hong, Steve Hammond, Chris Vervaet, Thomas De Beer*

1:55 Paper 565e: Identification of Key/Non-Key Process and Model Parameters of Polishing Chromatography, Primary Containers and Autoinjectors Using Mechanistic Models — ***Pablo A. Rolandi***, *Fabrice Schlegel*

2:15 Paper 565f: In-Situ Agglomeration Measurement During KDP Crystallization Based on Double-View Image Analysis — *Yan Huo,* ***Tao Liu***, *Cai Y. Ma, Xue Z. Wang*

2:35 Paper 565g: Progress in Industrial Implementation of Optical Coherence Tomography (OCT) for Real-Time Evaluation of Pharmaceutical Coating Processes — ***Patrick R. Wahl***, *Matthias Wolfgang, Anna Peter, Andrea V. Raffa, Phillip Clarke, Stephan Sacher, Johannes G. Khinast*

2:55 Concluding Remarks

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(566) Probing and Understanding Microbiomes and Microbial Communities
Wednesday, Nov 1, 12:30 PM
MCC, 205A/B

Ophelia S. Venturelli, Chair

Sponsored by:
Microbiomes and Microbial Communities

12:30 Paper 566a: Micro-Droplet-Enabled Co-Cultivation, Isolation, And Interaction Characterization of Microbial Communities — ***Xiaoxia (Nina) Lin***

12:52 Paper 566b: Metabolic Modeling of Microbial Communities — ***Costas D. Maranas***

1:14 Paper 566c: In-Vitro Fermentation to Understand Healthy and Stressed Gut Microbiome Metabolism — ***Laurel A. Doherty***, *Ida Pantoja-Feliciano, Steven Arcidiacono, Katherine Kensil, Kenneth Racicot, Jason W. Soares*

1:36 Paper 566d: Phylogenetic and Functional Profiling of the Microbiome Associated with a Phytoremediation System Targeting Air Quality in the Built Environment — *Jayamary Divya Ravichandar, Anna Dyson,* ***Cynthia H. Collins***

1:58 Paper 566e: Mechanical Principles of Biofilm Formation Revealed by Single-Cell Resolution Imaging of *V. cholerae* Biofilms — ***Jing Yan***, *Ned Wingreen, Bonnie Bassler, Howard A. Stone*

2:20 Paper 566f: Localization of Matrix Production Reveals *B. subtilis* Biofilm Growth Mechanics — ***Siddarth Srinivasan***, *Madhav Mani, Shmuel Rubinstein*

2:42 Paper 566g: Development and Characterization of a Promoter Library for Probiotic *E. coli* Nissle Using a High-Throughput Barcoding Approach — ***Nathan Crook***, *Zevin Condiotte, Gautam Dantas*

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(567) Process Intensification Through the Application of Microreactors and Membrane Reactors
Wednesday, Nov 1, 12:30 PM
MCC, 101E

Matthaeus Siebenhofer, Chair
Patrick Heider, Co-Chair

Sponsored by:
Process Intensification & Microprocess Engineering

12:30 Paper 567a: Comparative Study of a Hybrid Adsorptive-Membrane Reactor (HAMR) with a Membrane Reactor/Adsorptive Reactor Sequence — ***Secgin Karagoz***, *Theodore Tsotsis, Vasilios Manousiouthakis*

12:49 Paper 567b: Zeolite Membrane Reactor for High-Temperature Isobutane Dehydrogenation Reaction: Effects of Membrane Properties and Operating Conditions — *Shailesh Dangwal, Ruochen Liu,* ***Seok-Jhin Kim***

1:08 Paper 567c: IDEAS as a Process Intensification Tool Applied to Process Networks Containing Membrane Reactors — ***Patricia Pichardo***, *Vasilios Manousiouthakis*

1:27 Paper 567d: Additive Manufacturing for Process Intensification: Tailor-Made Design of Catalyst Supports for Single-Phase and Multiphase Reaction Systems — ***Hannsjörg Freund***, *Markus Lämmermann, Corinna Busse, Wilhelm Schwieger*

1:46 Paper 567e: Light Absorption Efficiency of Gas-Liquid Continuous Flow Microreactors Illuminated by Visible LED Light Sources
— *Anca Roibu, Tom Van Gerven,* ***Simon Kuhn***

2:05 Paper 567f: Fast Mixing, Ketimine Additions, and the Application of Flow Chemistry to Verubecestat
— ***John R. Naber****, David A. Thaisrivongs, Jonathan P. McMullen*

2:24 Paper 567g: Synthesizing High-Selectivity Bromobutyl Rubber by a Microreactor System — ***Pei Xie****, Kai Wang, Guangsheng Luo*

2:43 Paper 567h: Modeling and Optimization of a Two-Dimensional Tubular Reactor for an Exothermic Reaction — ***Soojin Kwon****, Sungwon Hwang*

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(568) Process Scale-Up Techniques
Wednesday, Nov 1, 12:30 PM
MCC, 102C

Vaibhav Kelkar, Chair
Shweta Karwa, Co-Chair

Sponsored by: Pilot Plants

12:30 Paper 568a: Liquid-Liquid Extraction: A Simplified View of a Complex Process
— *Jacob H. Arredondo,* ***Timothy Threatt****, Jonathan H. Worstell*

12:55 Paper 568b: The Inside Story of an Extractive Distillation Column: Process Modelling-Based Scale-Up with Plant Data in a Debottlenecking Case Study — ***Sekhar Babu Mamilla****, Antonio Matarredona*

1:20 Paper 568c: Applying CFD Towards Defining Crystallisation Scale-Up Strategy — ***Justine Forkin****,* ***Justin O'Sullivan***

1:45 Paper 568d: Lab-Scale Experimental Workflow to De-Risk Production Equipment Change for Filtration and Drying of Active Pharmaceutical Ingredients
— *Claire MacLeod,* ***Caroline Ainsworth****, Lucie Miller-Potucka, Anna Parsons, Alexandra Parker, David Wilson*

2:10 Paper 568e: Residence Time Estimative in a Thermal Cracking Reactor of Triglycerides
— *Bruna L. M. Frainer,* ***Vinicyus R. Wiggers****, Edésio L. Simionatto, Laércio Ender, Selene M. A. G. Ulson de Souza, Antônio A. Ulson de Souza, Henry F. Meier*

2:35 Paper 568f: Multiscale Approach to the Design of a Trickle-Bed Reactor
— ***Vaibhav Kelkar****, Sanjeev M. Rao, Debashis Chakraborty, Jorge Jimenez*

(569) Protein Engineering II: Combinatorial Techniques
Wednesday, Nov 1, 12:30 PM
MCC, 207A/B

Amy J. Karlsson, Chair
Zengyi Shao, Co-Chair

Sponsored by: Bioengineering

12:30 Paper 569a: Mutual Information to Inform Protein Library Design
— ***George Markou****, Casim A. Sarkar*

12:48 Paper 569b: Blueprints for Diversifying Small Protein Scaffolds in the Context of Multiple Secondary Structures — ***Daniel R. Woldring****, Max A. Kruziki, Benjamin J. Hackel*

1:06 Paper 569c: A Structure-Based High-Throughput Screening Method for Multi-Step Enzymatic Reactions Using Optically Guided Mass Spectrometry Profiling of Microbial Colonies
— ***Tong Si****, Bin Li, Troy J. Comi, Huimin Zhao, Jonathan V. Sweedler*

1:24 Paper 569d: Yeast Surface Display of Full-Length Human Tau for Combinatorial Antibody Profiling
— *Shiyao Wang,* ***Yongku Cho***

1:42 Paper 569e: Saturation Mutagenesis Panning Libraries Enable Activity and Specificity Modulation of Microcin J25 — ***Seth Ritter****, Mike Yang, Yiannis N. Kaznessis, Benjamin J. Hackel*

2:00 Paper 569f: Accessing the Location-Dependent Effects of Unnatural Amino Acids on Protein Expression and Activity with Cell-Free Protein Synthesis-Facilitated Rapid Screening — ***Bradley C. Bundy****, Song-Min Schinn, William Bradley, Ashtyn Groesbeck, Jeffrey C. Wu, Andrew Broadbent*

2:18 Paper 569g: RNA-Programmed DNA Methylation — ***Marc Ostermeier***

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(570) Protein Structure, Function, and Stability II: Aggregation & Disease
Wednesday, Nov 1, 12:30 PM
MCC, 208A

Robert Luo, Chair
Seongkyu Yoon, Co-Chair
Han Li, Co-Chair

Sponsored by: Bioengineering

12:30 Paper 570a: Engineering a Self-Assembling Peptide System Derived from Beta-Amyloid — ***Jason Candreva****, Edward Chau, Jin Ryoun Kim*

12:48 Paper 570b: Competition Between Ligands: How Retinol-Binding Protein and Beta-Amyloid Compete for Binding to Transthyretin
— ***Parth Mangrolia****, Chandler Est, Regina M. Murphy*

1:06 Paper 570c: Understanding the Role of Glycine in Amyloid Protein Aggregation Through Rationally Designed Protein Sequences
— ***S. Zeb Vance****, Rachel Hall, Jamie Crawford, Gram L. Booth, Christa N. Hestekin, Melissa A. Moss*

1:24 Paper 570d: N-Terminal Hypothesis for Alzheimer's Disease: Analyzing Dimers of a β-Peptide and Its Protective and Causative Mutants
— ***Bhanushee Sharma****, Srivathsan V. Ranganathan, Mirco Sorci, Christopher Lennon, James Van Deventer, Annalisa Scimemi, Georges Belfort*

1:42 Paper 570e: Computational Modeling of Amyloid Aggregation Kinetics to Gain Insights into the Effect of Ions on Amyloid Aggregation
— ***Aditi Sharma****, Harrison B. Rose, Yury O. Chernoff, Sven H. Behrens, Andreas S. Bommarius*

2:00 Paper 570f: Human Islet Amyloid Polypeptide: Identifying Early-Stage Aggregation Mechanisms Through Molecular Simulation — ***Ashley Guo****, Juan de Pablo*

2:18 Paper 570g: The Role of Cholesterol in Membrane Protein Activity — ***Anne S. Robinson***

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(571) Reaction Engineering for Combustion and Pyrolysis
Wednesday, Nov 1, 12:30 PM
MCC, L100C

C. Franklin Goldsmith, Chair
Bihter Padak, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

12:30 Paper 571a: Kinetics of the Thermal Decomposition of Carbonyl Sulfide — ***Marko R. Djokic****, Ruben Van de Vijver, Manjunath Patil, Guy B. Marin, Kevin M. Van Geem*

12:52 Paper 571b: A Cylindrical Formulation of the One-Dimensional Turbulence (ODT) Model for Turbulent Jet Flames — ***David O. Lignell****, Victoria B. Lansinger, Alan Kerstein*

1:14 Paper 571c: Automated Transition State Theory Calculation of Hydrogen Abstraction from Novel Biofuels
— ***Nathan Harms****, Richard H. West*

1:36 Paper 571d: First-Principles-Based Automated Kinetic Model Generation Using On-the-Fly Ab-Initio Calculations — ***Ruben Van de Vijver****, Guy B. Marin, Kevin M. Van Geem*

1:58 Paper 571e: Quantifying the Catalytic Effect of Calcium on Initiation During Cellulose Pyrolysis
— ***Gregory G. Facas****, Cheng Zhu, Matthew Neurock, Paul J. Dauenhauer*

2:20 Paper 571f: Development of a Micro-Kinetic Model of Soot for Ethylene Flames — ***Srivathsan Sundar****, Preeti Aghalayam, Satyanarayanan R. Chakravarthy*

2:42 Paper 571g: Artificial Neural Networks for Flare Modeling and Set Point Determination
— ***Vijaya Damodara****, Daniel H. Chen, Helen H. Lou, Arokiaraj Alphones, Christopher B. Martin, Xianchang Li*

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(572) Safety and Sustainability Best Practices
Wednesday, Nov 1, 12:30 PM
MCC, 101C

Konstantinos E. Kakosimos, Chair
William M. Barrett, Co-Chair
Hebab Quazi, Co-Chair
Eric Peterson, Co-Chair

Sponsored by: General

12:30 Paper 572a: Methodologies for Life-Cycle Inventory Generation of Chemicals and Their Implication on the Life-Cycle Impact Assessment Results — ***Abhijeet Parvatker****, Matthew J. Eckelman*

12:50 Paper 572b: A Novel Dynamic Routing Model for the Transportation of Hazardous Materials Under Uncertainties and Potential Shipping Delays — ***Honglin Qu****, Sujing Wang, Qiang Xu*

1:10 Paper 572c: Integrated Sustainable Design Approach for Assessing Inherent Process Safety During Early Stage of Design
— ***Monzure-Khoda Kazi****, Fadwa T. Eljack, Vasiliki Kazantzi*

1:30 Paper 572d: Effect of Dynamic Operation Behavior on Quantitative Risk Assessment for Gas Treatment Unit of Gas-Oil Separation Plant
— ***Seolin Shin****, Usama Ahmed, Chonghun Han*

1:50 Paper 572e: Unsteady Kinetics and Thermodynamics Through TFE Pyrolysis Production Process Based upon Inherent Safety Assessment
— ***Yangmei Qin****, Zeyi Xiao, Shimeng Guo, Jiying Zeng*

2:10 Paper 572f: Source-to-Customer Integration for Sustainability
— ***Andrew W. Sloley***

(573) Special Session: Celebrating Prof. Mori's Career-Long Accomplishments
Wednesday, Nov 1, 12:30 PM
MCC, 200I

Nobusuke Kobayashi, Chair
L.-S Fan, Co-Chair

Sponsored by: Fluidization and Fluid-Particle Systems

12:30 Professor Shigekatsu Mori: An Outstanding Scholar, Researcher, Engineer, and Educator

12:35 Paper 573a: Developments of Coal-Fired Power Generation Processes in Japan After the First Oil Crisis (1973)
— ***Shigekatsu Mori***

12:55 Paper 573b: Selected Topics in Fluidization Fundamentals and Fluidized-Bed Applications: A Presentation Honoring Prof. Shigekatsu Mori — ***Thomas Ho***

1:15 Paper 573c: Fluidized-Bed Drying Process Based on Self-Heat Recuperation Technology
— ***Atsushi Tsutsumi****, Lu Chen, Hiroyuki Mizuno, Yasuki Kansha*

1:35 Paper 573d: The Role of Pressure Balance in Nonmechanical Device Design — ***T. M. Knowlton***

1:55 Paper 573e: Carbon Fiber Reclamation from CFRP Waste
— ***Hiroshi Moritomi***

2:15 Paper 573f: A Nature-Inspired Approach to Aid the Understanding and Improve the Performance of Fluidized Beds — ***Marc-Olivier Coppens***

2:35 Concluding Remarks

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(574) Thermophysical Properties and Phase Behavior IV: Theory and Equations of State
Wednesday, Nov 1, 12:30 PM
MCC, L100J

Eric Jankowski, Chair
Sanket Deshmukh, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

12:30 Paper 574a: Predicting Vapor-Liquid Equilibria with Augmented Ab-Initio Potentials — *Maryna Vlasiuk,* ***Richard J. Sadus***

12:46 Paper 574b: New Vapor Pressure Prediction with Improved Thermodynamic Consistency Using the Riedel Equation — ***Joseph W. Hogge****, Neil Giles, Richard L. Rowley, Thomas A. Knotts IV, W. Vincent Wilding*

1:02 Paper 574c: Solvent Screening and Pure Component Thermophysical Property Prediction for Pharmaceutical Process Design — ***Getachew S. Molla****, Łukasz Ruszczynski, Jens Abildskov, Gürkan Sin*

1:18 Paper 574d: A Two-Structure Equation of State for Super-Cooled and Stretched Light and Heavy Water
— ***Michal Duška****, Jan Hruby, Frédéric Caupin, Mikhail A. Anisimov*

1:34 Paper 574e: Can Molecular Simulations Predict the Binary Interaction Parameters of the Activity Coefficient Models?
— ***Ashwin Ravichandran****, Rajesh Khare, Chau-Chyun Chen*

1:50 Paper 574f: A Wertheim Activity Coefficient Model for Associating Mixtures — ***Aseel M. Bala****, William G. Killian, Jackson A. Storer, James E. Jackson, Paul M. Mathias, Navin Patel, Timothy C. Frank, Dung T. Vu, Eric L. Cheluget, Carl T. Lira*

2:06 Paper 574g: Understanding the Role of Intermolecular Forces in Molecular-Based Equations of State: 20 Years of the Soft-SAFT Equation
— ***Lourdes F. Vega****, Fèlix Llovell, Felipe J. Blas, Oriol Vilaseca, Joao A. P. Coutinho, Jordi Torné*

2:22 Paper 196b: Coarse-Grained Modeling of Polymer Materials in Molecular Simulations with SAFT-γ Mie Corresponding States Correlation Specified Potentials — ***Amulya Pervaje****, Saad A. Khan, Erik E. Santiso*

2:38 Paper 574h: New SAFT EOS for Electrolyte Solution — *Reza Shahryari,* ***Mohammad Reza Dehghani***

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(575) Thermophysical Properties of Biological Systems
Wednesday, Nov 1, 12:30 PM
MCC, L100I

Phanourios Tamamis, Chair
Thomas A. Knotts IV, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

12:30 Paper 575a: Controlling Vesicle Shape by Adsorption of a Semiflexible Polymer — *Bing Li,* ***Steven M. Abel***

12:48 Paper 575b: Polymer-Induced Restructuring in the Gut
— ***Sujit S. Datta****, Asher Preska Steinberg, Rustem Ismagilov*

1:06 Paper 575c: Multicomplex Formation in the Presence of Polymer Crowders Mimicking In-Cell Environment — ***Vahid Rahmanian****, Young C. Kim, Jeetain Mittal*

1:24 Paper 575d: Effect of Palmitoylation in Membrane Proteins at the Blood-Brain Barrier Interface
— ***Nandhini Rajagopal****, Flaviyan Jerome Irudayanathan, Shikha Nangia*

1:42 Paper 575e: Determining the Limitations of Processive Polysaccharide Deconstruction by Glycoside Hydrolases
— *Suvamay Jana, Brandon C. Knott, Gregg T. Beckham,* ***Christina M. Payne***

2:00 Paper 575f: Computational Design of Novel Self-Assembling Peptide Biomaterials Based on an Amyloid-Forming Motif from the Adenovirus Fiber Shaft — ***Sai Vamshi R. Jonnalagadda****, Graziano Deidda, Eirini Ornithopoulou, Asuka Orr, Anna Mitraki, Phanourios Tamamis*

2:18 Paper 575g: Conformational Changes of 2'-Hydroxybiphenyl-2-Sulfinate Desulfinase — ***Yue Yu****, Christina M. Payne*

2:36 Paper 575h: Chromatin Folding via Coarse-Grained Multiscale Simulation — ***Joshua Lequieu****, Andres Cordoba, Joshua Moller, Juan de Pablo*

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(576) Thin-Film Block Copolymer Self-Assembly and Morphology
Wednesday, Nov 1, 12:30 PM
MCC, 211B

Muzhou Wang, Chair
Daniel T. Hallinan Jr., Co-Chair

Sponsored by: Polymers

12:30 Paper 576a: Quantitative Three-Dimensional Morphological Characterization of Block Copolymer Films Enabled by Directed Self-Assembly — ***Paul F. Nealey***

1:00 Paper 576b: Examination of Line Edge Roughness of Directed Self-Assembled Block Copolymers: A Coarse-Grained Molecular Dynamics Study — ***Shubham Pinge****, Durairaj Baskaran, Munirathna Padmanaban, Yong Lak Joo*

1:15 Paper 576c: Atomistic Simulations of Ion Transport in PS-b-P2VP-Functionalized Lamellae
— ***Weiwei Chu****, Yamil J. Colón, Juan de Pablo*

1:30 Paper 576d: Performance of the Novel Ultra-Thin Proton-Exchange Membrane Based on Poly(arylene ether sulfone)s for PEMFCs — ***Yang Zhao****, Xue Li, Xiaofeng Xie*

1:45 Paper 576e: The Consequence of Morphology on Conductivity for Bolaamphiphiles — ***Mayank Misra****, Christian Nowak, Yangyang Sun, Fernando Escobedo*

2:00 Paper 576f: Mechanical and Structural Analyses of Toughened Syndiotactic Polypropylene Gels: Effects of Gel-Preparation Temperature
— ***Fuyuaki Endo****, Ryusuke Okoshi, Naruki Kurokawa, Tomoki Maeda, Atsushi Hotta*

2:15 Paper 576g: Chemically Cross-Linked Poly(2-Hydroxyethyl Methacrylate)-Supported Deep Eutectic Solvent Gel Electrolytes — ***Huan Qin****, Matthew J. Panzer*

2:30 Paper 576h: Ultrasonic Synthesis of Temperature-Responsive Copolymer and Its Characterization
— ***Masaki Kubo****, Tomoyuki Koshimura, Takao Tsukada*

2:45 Paper 576i: Atomic-Level Comparisons of LCST Transition in Thermo-Sensitive Polymers
— ***Yaxin An****, Karteek Bejagam, Samrendra Singh, Sanket A. Deshmukh*

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(577) Turbulent and Reactive Flows
Wednesday, Nov 1, 12:30 PM
Hilton, Marquette I/II/III/VIII/IX

Li Xi, Chair
De-Wei Yin, Co-Chair

Sponsored by: Fluid Mechanics

12:30 Paper 577a: Quantitative Prediction of Industrial Turbulent Processes in Stirred-Tank Reactors (Invited) — ***Minye Liu***

1:00 Paper 577b: Passive Scalar Mixing in Anisotropic Turbulence from Line Sources — ***Quoc T. Nguyen****, Dimitrios V. Papavassiliou*

1:15 Paper 577c: Dynamics and Structures of Viscoelastic Turbulence in Transitional Channel Flow
— ***Ashwin Shekar****, Sung-Ning Wang, Michael D. Graham*

1:30 Paper 577d: Polymer Effects on the Development and Bursting of Turbulent Vortices: Implication on High-Extent Drag Reduction — *Lu Zhu, Xue Bai,* ***Li Xi***

1:45 Paper 577e: Turbulent Pipe Flow Drag Reduction Using Dilute Solutions of High-Molecular-Weight Polymers: Experimental Studies Elucidating the Role of the Highest Molecular-Weight Fractions Using Well-Characterized Polymer Systems
— *Talal D. H. Al Shamrani, Davis A. Jacob, Brian D. Jones, Willie E. Rochefort,* ***Travis W. Walker***

2:00 Paper 577f: Macroscale Insensitivity of Type-B Drag Reduction by Two Biopolymers
— ***Preetinder S. Virk***

2:15 Paper 577g: Euler-Euler and Euler-Lagrange Simulations of Heavy Particles Clustering in Homogeneously Sheared Gas — ***Mohamed H. Kasbaoui***, *Olivier Desjardins, Donald L. Koch*

2:30 Paper 577h: Breakage of Single Drops and Bubbles in a Turbulent 2-D Orifice Flow — ***Derrick I. Ko***, *Richard V. Calabrese*

2:45 Paper 577i: On the Influence of Spanwise Boundary Conditions on the Large Eddy Simulation of the Flow Past a Single Cylinder — *Barbara L. Silva, Matheus R. Barbieri,* ***Jonathan Utzig***, *Henry F. Meier*

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(578) Unconventionals: Shale Gas, LNG, CNG, and LPG
Wednesday, Nov 1, 12:30 PM
MCC, 200A

Sheima J. Khatib, Chair
Belma Demirel, Co-Chair

Sponsored by:
Alternate Fuels and New Technology

12:30 Paper 578a: Natural Gas Liquids (NGL): To Fractionate or Not to Fractionate at the Gas Processing Plant? — ***Bijal Gangar***, *Ali A. Pilehvari*

12:48 Paper 578b: LNG Market and Technology — ***Jeffrey Zhang***

1:06 Paper 578c: Visual Measurements of Hydrocarbon Freeze-out Temperature in LNG Mixtures: Experimental Design — ***Arman Siahvashi***, *Saif Al-Ghafri, Eric F. May*

1:24 Paper 578d: Plant-Wide Modeling, Techno-Economic Analysis and Optimization of the Shale Gas-to-Dimethyl Ether (DME) Process via Direct and Indirect Synthesis Route — ***Chirag Mevawala***, *Yuan Jiang, Debangsu Bhattacharyya*

1:42 Paper 578e: New Thermophysical Properties Measurements of Complex Mixtures Relevant to Liquefied Natural Gas (LNG) Processing — ***Saif Al-Ghafri***, *Masoumeh Akhfash, Arash Arami-Niya, Sofia Mylona, Kumarini Seneviratne, Fuyu Jiao, Jordan Oakley, Thomas Hughes, Michael L. Johns, Eric F. May*

2:00 Paper 578f: Numerical Investigation for Heat Transfer of Supercritical Methane Heated in a Horizontal Circular Tube — ***Binhui Ruan***, *Wensheng Lin*

2:18 Paper 578g: Study on Ice Storage System Based on Cold Energy Utilization in LCNG Fueling Stations — ***Siyue Zhao***, *Wensheng Lin, Wei Qiu*

(579) USA-China Progress in Biomass Conversion Technologies I
Wednesday, Nov 1, 12:30 PM
MCC, 200E

Shijie Liu, Chair
Xinshu Zhuang, Co-Chair

Sponsored by:
Biorefinery Technologies for Forest-Based Lignocellulosic Biomass

12:30 Paper 579a: Preparation and Characterization of Co-Cu-Ga/ZrO_2-Al_2O_3 Catalyst for Higher Alcohol Synthesis from Syngas — ***Gaofeng Chen***, ***Tingzhou Lei***, ***Zhiwei Wang***

12:52 Paper 579b: Conversion of Gluconate and Glycerol to Ethanol Using the Recombinant *Klebsiella oxytoca* Strains — ***Weiyi Tao***, *Hui Lin, He Huang,* ***Zhiliang (Julia) Fan***

1:14 Paper 579c: Ammonia Stripping for Enhanced Biomethanization of Chicken Manure — ***Ronghou Liu***

1:36 Paper 579d: Role of O in Ru Catalyst in Hydrodeoxygenation of Furfural — ***Weiqing Zheng***, *Konstantinos A. Goulas, Ayman M. Karim, Prashant Kumar, K. Andre Mkhoyan, Michael Tsapatsis, Dionisios G. Vlachos*

1:58 Paper 579e: Optimization for Technological Conditions of Magnetic Ferric Oxide/SO_4^{2-} Biomass-Based Solid Acid–Catalyzed Hydrolysis Corn Straw to Prepare Levulinic Acid Using Response Surface Methodology — ***Xueqin Li***, ***Tingzhou Lei***, ***Zhiwei Wang***, *Gaofeng Chen, Haiyan Xu, Qian Guan, Zijie Li*

2:20 Paper 579f: Supercritical CO_2 Pretreatment of Wheat Straw: Hydrolysis Performance, Enzymatic Yields and Comprehensive Mass Balances — ***Ana R. C. Morais***, *Rafal M. Lukasik*

2:42 Paper 579g: Conversion of Biomass to Microbial Lipids for Biofuels — ***Zongbao Zhao***

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(580) Water Treatment, Desalination, and Reuse II
Wednesday, Nov 1, 12:30 PM
MCC, M100H

Jamie Hestekin, Co-Chair
Ngoc Bui, Co-Chair
Oishi Sanyal, Co-Chair
Isabel Escobar, Co-Chair

Sponsored by:
Membrane-Based Separations

12:30 Paper 580a: Metal-Organic Frameworks UiO-66 and MIL-125 Nanoparticles Enhance the Performance of Thin-Film Nanocomposite Membrane for Water Desalination — ***Mohammed Kadhom***, *Baolin Deng*

12:50 Paper 580b: The Time Evolution of Fouling Development upon Design Aspects of Direct-Flow Filtration — ***Qian Xu***, *Robert Field*

1:10 Paper 580c: Overcoming Operating Pressure Barrier in High-Recovery Membrane Desalination via Hybrid RO-NF Processes — ***Anditya Rahardianto***, *Yoram Cohen*

1:30 Paper 580d: Development and Performance of a Silver Nanoparticle–Impregnated Reusable Anti-Biofouling Membrane in a Continuous Cross-Flow Membrane Module — *Pritam Biswas,* ***Rajdip Bandyopadhyaya***

1:50 Paper 580e: Performance of a Cost-Effective Micro-Scale Biochar/PSF Mixed-Matrix Hollow Fiber Membrane in the Treatment of Methylene Blue Simulated Wastewater — *He Jinsong,* ***Chen J. Paul***

2:10 Paper 580f: Treating Poultry Processing Wastewaters by Ultrafiltration — ***S. Ranil Wickramasinghe***, *Yu-Hsuan Chiao, Kamyar Sardari*

2:30 Paper 580g: Ceramic Hollow Fiber–Supported Metal-Organic Framework UiO-66 for Enhanced Adsorptive Separations — ***Chenghong WANG***

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(581) Award Session: AES Electrophoresis Society (Invited Talks)
Wednesday, Nov 1, 1:15 PM
Hilton, Marquette IV/V/VI/VII

Rodrigo Martinez-Duarte, Chair

Sponsored by: 2017 Annual Meeting of the AES Electrophoresis Society

1:15 Paper 581a: 3D Dielectrophoresis — ***Michael P. Hughes***

1:45 Paper 581b: Electrical Manipulation of Cells for Biology and Medicine — ***Joel Voldman***

2:15 Paper 581c: Dielectrophoresis Shows That Regular Potassium Transport Controls the Circadian Electrophysiological Rhythm in Human Red Blood Cells — ***Fatima H. Labeed***

2:45 Paper 581d: Isomotive Dielectrophoresis: Design Considerations and Scaling Laws — ***Stuart J. Williams***

3:15 Paper 581e: Exploring the '2nd Frontier' of Dielectrophoresis and Its Application in the Biomedical Sciences — ***Ronald Pethig***

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(582) Poster Session: Catalysis and Reaction Engineering (CRE) Division
Wednesday, Nov 1, 3:15 PM
MCC, Exhibit Hall B

Joshua Snyder, Chair
Hari Nair, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

■ BIOMASS/BIO-BASED CATALYSIS

Paper 582a: Hydrolysis of Corncob Using a Modified Carbon-Based Solid-Acid Catalyst — ***Wei Qi***

Paper 582b: Preparation of Biodiesel from Waste Cooking Oil via Lithium Metasilicate-Catalyzed Transesterification Reaction — *Gina YC Chen, Dai-Ying Lin, Duu-Jong Lee,* ***Bing-Hung Chen***

Paper 582c: Hydrothermal Co-Carbonization (HTCC) of Coal-Biomass Blend — *Akbar Saba, Pretom Saha,* ***M. Toufiq Reza***

Paper 582d: Tunable Oleo-Furan Surfactants via Acylation of Biomass-Derived Furans — ***Kristeen Esther Joseph***, *Dae Sung Park, Christoph Krumm, Michael Tsapatsis, Raul F. Lobo, Dionisios G. Vlachos, Paul J. Dauenhauer*

Paper 582e: Catalytic Upgradation of Biomass-Derived Bio-Oil by C-C Coupling of Phenolic Compounds with Light Oxygenates — ***Gul Afreen***, *Tanmoy Patra, Ratan Mohan, Sreedevi Upadhyayula*

Paper 582f: Development of High-Performance Heterogeneous Catalysts for Valorization of Biogenic Chemicals — ***Tomoo Mizugaki***, *Kohei Uesugi, Kodai Nitta, Zen Maeno, Takato Mitsudome, Koichiro Jitsukawa, Kiyotomi Kaneda*

Paper 582g: Metal H-Beta Zeolite Catalytic Upgrading of Bio-Crude Oil Derived from Hydrothermal Liquefaction of Algae — ***Zheng Cui***, *Feng Cheng, Neil Paz, Umakanta Jena, Catherine E. Brewer, Tanner Schaub*

Paper 582i: Catalytic Depolymerization of Lignin into Value-Added Chemicals over $CuO(X)MgAlO_y$ Catalysts in Supercritical Ethanol — *Soyeon Jeong, Seungdo Yang,* ***Do Heui Kim***

Paper 582j: Investigation of Imogolite Nanotubes as a Catalyst for Biomass Conversion — ***Nathaniel Olson***, *Nicholas Brunelli*

Paper 582k: Thermodynamic and Kinetic Analysis of γ-Valerolactone Ring Opening in Multiphase Reactors — ***Xinlei Huang***, *Zijian Wang, Jesse Q. Bond*

Paper 582l: Integrating Hydride Donor Regeneration with Size-Selective Capsules for Efficient and Sustainable Biohydrogenation — ***Shaohua Zhang***, *Zhongyi Jiang,* ***Jiafu Shi***

■ HETEROGENEOUS CATALYSIS (LARGE MOLECULE)

Paper 582m: Selective Dehydration of Polyols on Copper-Modified Brønsted Acid Support — ***Yan Cheng***, *Brent H. Shanks*

Paper 582n: Kinetic Study of Enzyme-Catalyzed Phenol and Its Derivatives Oxidative Coupling Products — ***Kaidong Wang***, *Guoqiang Jiang, Zheng Liu*

Paper 582o: Effect of Dehydrating Agent in Cu/Y-Zeolite Catalyst on Oxidative Carbonylation of Methanol for Dimethyl Carbonate Synthesis — ***Dong-Ho Lee***, *Je-Min Woo, Jung Yoon Seo, Hyunuk Kim, Young Cheol Park, Jong-Ho Moon*

Paper 582p: CFD Simulation About Isobutane Alkylation Catalyzed by Ionic Liquid in Cyclone Reactor — ***Shuiqiang Duan***, *Mengzijing Chen, Rui Zhang, Xianghai Meng, Haiyan Liu, Zhenbo Wang, Zhichang Liu*

Paper 582q: Microreactor Techniques for Analysis of Complex Reactions — ***Saurabh Maduskar***, *Paul J. Dauenhauer*

Paper 582r: Membrane Reformers: Optimization of Catalysts and Membranes for Production of Ultra-Pure Hydrogen Through Steam Reforming of Methanol — ***Richa Sharma,*** *Amit Kumar, Rajesh Kumar Upadhyay*

Paper 582s: Fe- and Zn-Promoted Mo/ZSM-5 Catalyst for the Conversion of Ethane into Aromatic Products — ***Brandon Robinson***, *Xinwei Bai, Anupam Samanta, Victor Abdelsayed, Dushyant Shekhawat, John Hu*

Paper 582t: Reforming of Methanol Aqueous Solution Use of Superheated Liquid-Film Concept — ***Daisuke Kobayashi***, *Shin Kobayashi, Masakazu Naya, Atsushi Shono, Katsuto Otake, Yasukazu Saito*

Paper 582u: Methanol to Propylene Conversion: Recent Development Trends — ***Shakeel Ahmed***, *Mohammad Ashraf Ali, Nadhir Al-Baghli, Zuhair Omar Malaibari*

Paper 582v: Resin-Based Solid-Acid Catalyst for Dehydration of Fructose to HMF — ***Aamena Parulkar***, *Mariah Whitaker, Rutuja Joshi, Nicholas Brunelli*

Paper 582w: Optimizing ZSM-11 Catalysts for Methanol-to-Hydrocarbon Reactions — ***Yufeng Shen***, *Thuy T. Le, Jeffrey D. Rimer*

Paper 582x: Selective Glucose Isomerization to Fructose Using Heterogeneous Amine Catalysts — ***Nitish Deshpande***, *Lagnajit Pattanaik, Mariah Whitaker, Nicholas Brunelli*

Paper 582y: Group IV and V Periodic Trends in Olefin Epoxidation: Effects of Electronic Structure and Local Environment — ***Daniel T. Bregante***, *Nicholas E. Thornburg, Justin M. Notestein, David W. Flaherty*

Paper 582z: Mechanistic and Spectroscopic Evidence for Reactive Intermediate Structures During C-O Bond Rupture in Oxygenates over Metal Phosphide Clusters — *Megan E. Witzke, Abdulrahman S. Almithn, Christian L. Coonrod, Mark D. Triezenberg, David D. Hibbitts,* ***David W. Flaherty***

Paper 582aa: Utilizing Solvent Effects Within Heterogeneous Catalysts for Selective Production of 5-Hydroxymethylfurfural — ***Mariah Whitaker***, *Lagnajit Pattanaik, Kory Sherman, Rutuja Joshi, Nicholas Brunelli*

Paper 582ab: Understanding the Effect of Alloying Pd and Sn on Direct Synthesis of H_2O_2 — ***Pranjali Priyadarshini***, *Neil M. Wilson, Jason S. Adams, David W. Flaherty*

Paper 582ac: Optimal Control of a Fluid Catalytic Cracking Unit — ***Arturo Ortiz-Arroyo***, *Angel Castro, Fernando Pérez*

Paper 582ad: Enzymatic Cascade Reactions for Synthesis of High-Value Products in a Multiphase System — ***Jens Johannsen***, *Georg Fieg, Thomas Waluga*

Paper 582ae: Hydrogenation of Phenol to Cyclohexanone via Tubular Nanofiber-Supported Catalyst — ***Lin Pan***

Paper 582af: Silica Gel–Confined Carboxylic Functionalized Imidazolium Salt for One-Step Catalytic Hydration of Ethylene Oxide — ***Qian Su***, *Weiguo Cheng, Suojiang Zhang*

Paper 582ag: Catalytic Aqueous-Phase Reforming of Methanol to Produce Hydrogen — ***Irene Coronado***

Paper 582ah: Glycerol Valorization to Oligomers of Glycerol by Etherification over Supported Sr and Ca Catalysts — *Yo-Ru Chen, Hsiang-Ming Wu,* ***Bing-Hung Chen***

Paper 582aj: Positive Synergy in Bimetallic WZr Mesoporous Silicates for Ethanol Conversion Reactions — ***Hongda Zhu***, *Anand Ramanathan, Jian-Feng Wu, Bala Subramaniam*

Paper 582ak: The Role of External Acidity of Hierarchical ZSM-5 Zeolites in n-Heptane Catalytic Cracking — ***Xiaoxiao Zhang***, *Dangguo Cheng, Fengqiu Chen, Xiaoli Zhan*

Paper 582al: Catalytic Cracking of Light and Heavy Crude Oil Blends to Maximise Light Olefins: Impact of Conversion and Product Yields — ***Gnana Pragasam Singaravel***

Paper 582am: Kinetics of Resid Fluid Catalytic Cracking Using a Fixed Fluidized-Bed Reactor — ***Abdul Majed Al Katheeri***

Paper 582an: Assembly of Kaolin and SAPO-34 Catalyst Using Silica Sol as Binder by Spray Drying for Conversion of Methanol to Light Olefins in Fluidized-Bed Reactor: Effect of Ion Exchange Method — ***Sogand Aghamohammadi***, *Mohammad Haghighi, Alireza Ebrahimi*

Paper 582ao: Functionalized Metal–Organic Framework as a Biomimetic Heterogeneous Catalyst for Transfer Hydrogenation of Imines — ***Jingwen Chen***

Paper 582ap: Study on the Influence of Particle Size Distribution on the Solid-Liquid Reaction to Produce Sucrose Ester — *Maria F. Gutierrez, Andrea Suaza, Jose L. Rivera,* ***Alvaro Orjuela***

Paper 582aq: Acid Catalyst Coupling with Ionic Liquids to Catalyse C_4 Alkylation Process Synergistically — *Tao Zhang, Keting Jing, Yuan Zhang, Shuai Zhang, HongXia Li, Fei Zhou, Jing Hu, Yaling Li,* ***Shengwei Tang Sr.***

■ ELECTROCATALYSIS/ PHOTOCATALYSIS

Paper 582ar: Kinetics Studies on Redox Flow Battery Electrolytes — ***Tejal Sawant***, *James R. McKone*

Paper 582as: Direct Photocatalytic Reduction of Bicarbonate to Formate on Plasmonic Metallic Nanoparticles — *Hanqing Pan,* ***Keeniya-Gamalage-Gehan De-Silva***, *Michael D. Heagy, Sanchari Chowdhury*

Paper 582at: Engineering Metal/SnO_x Interfaces for Electrochemical CO_2 Reduction — ***Siwen Wang***, *Hongliang Xin*

Paper 582au: Mechanistic Insights into the Effect of Electrolyte Composition on the Electroreduction of Carbon Dioxide (CO_2) to C_1-C_2 Chemicals Using a Flow Electrolyzer — ***Sumit Verma***, *Paul J. A. Kenis*

Paper 582av: Gold Nanoparticle Clusters as Fenton Reaction Photocatalysts — ***Siddharth Agrawal***, *Michael P. Hoepfner, Swomitra Mohanty*

Paper 582aw: Interconnection of Spillover and Electrochromism at Tungsten Oxide — ***Rituja Patil***, *James R. McKone*

Paper 582cw: Evaluating the Surface Science of Photocatalytic Nitrogen Fixation — ***Avery Agles***, *Nathan James, Marta Hatzell*

■ COMPUTATIONAL CATALYSIS

Paper 582ax: Analyzing Reaction Networks and Pathway Kinetics via Metadynamics Simulations — ***Christopher Fu***, *Jim Pfaendtner*

Paper 582ay: An Integrated Workflow for Numerical Generation and Meshing of Packed Beds of Non-Spherical Particles: Applications in Chemical Reaction Engineering — ***Behnam Partopour***, *Anthony G. Dixon*

Paper 582az: First-Principles Studies of CO Oxidation on $MgAl_2O_4$-Supported Iridium Single Atoms — ***Jiamin Wang***, *Yubing Lu, Ayman M. Karim, Hongliang Xin*

Paper 582ba: Feature Engineering of Machine-Learning Models for Metal Oxides — ***Zheng Li***, *Hongliang Xin*

Paper 582bb: Electrode-Electrolyte Interfaces Probed by Quantum-Chemical Simulations and Machine Learning for Lithium-Ion Batteries — ***Noushin Omidvar***, *Hongliang Xin*

Paper 582bc: A DFT Study of CO Adsorption and Coverage on Co_7Pd_6 13 Atom Cluster — ***Anuradha Gundamaraju***

Paper 582bd: Microkinetic Modeling of Hydrogen Oxidation on Transition Metal Surfaces for SOFC Anode — ***Sarwar Hussain***

Paper 582be: Bifurcation Analysis of a Two-Dimensional Homogeneous Reactor Model — ***Zhe Sun***, *Vemuri Balakotaiah*

Paper 582bf: Studies on Redox Properties of Dual Metal-Substituted Ceria — ***Phanikumar Pentyala***, *Parag A. Deshpande*

Paper 582bg: Simulation of Adiabatic Trickle-Bed Reactor for Liquid-Phase Catalytic Exchange of Hydrogen Isotopes — ***Ran Wang***, *Feng Xin*

Paper 582bh: Development of a Micro-Kinetic Model of NO-CO Reaction over Gold Catalyst and Validation — *Anupam Abha, Vishnu S. Prasad,* ***Preeti Aghalayam***

■ CATALYST DEVELOPMENT/ SYNTHESIS

Paper 582bi: Incorporating Catalysts into Textile Substrates and Their Resulting Properties — ***Nicole Hoffman****, Natalie Pomerantz, Nick Dugan, Joe Rossin*

Paper 582bj: Spectroscopic and Kinetic Assessment of Sn Sites Incorporated into Chabazite Frameworks at Intracrystalline and Extracrystalline Locations — ***James W. Harris****, Wei-Chih Liao, John R. Di Iorio, Alisa M. Henry, Ta-Chung Ong, Aleix Comas-Vives, Christophe Copéret, Rajamani Gounder*

Paper 582bk: Zeolite Catalyst Design and Optimization: Impact of Synthesis Parameters on Crystal Properties — ***James Sutjianto,*** *Rui Li, Jeffrey Rimer*

Paper 582bl: Elucidating Zeolite Crystal Growth Mechanisms by Atomic Force Microscopy — ***Madhuresh K. Choudhary****, Manjesh Kumar, Jeffrey D. Rimer*

Paper 582bm: Production and Characterization of Boron Nitride Nanotubes from Reaction of Ammonia with Mixture of Boron and Iron Powders — ***Naime Aslı Sezgi****, Selin Noyan*

Paper 582bn: Crystallization of One-Dimensional Zeolites by Nonclassical Pathways: Perspectives on Nucleation and Crystal Growth — ***Rui Li****, James Sutjianto, Aseem Chawla, Jeffrey Rimer*

Paper 582bo: Tailoring the Morphology and Active Site Distribution of ZSM-5 Catalysts — ***Wei Qin****, Matthew Patton, Jeffrey Rimer*

Paper 582bp: Effects of Surfactant Concentration and Cosolvent on the Morphology of Hexagonal Mesoporous Silica — ***Yu-Wen Chen***

Paper 582bq: Crystal Structures, Electronic and Optical Properties of Few Single Monolayer of SnH —

Paper 582br: Knoevenagel Condensation over Ion-Exchanged Low-Silica Beta Zeolites: Their Catalytic Properties and Kinetic Analysis — ***Takahiko Moteki****, Masaru Ogura*

Paper 582bs: Reverse-Microemulsion Method–Prepared NiPt Catalysts for Methane Decomposition — ***Lu Zhou***

Paper 582bt: How pH Affects the Metal Dispersion on Silica-HMS, MCM-41 and SBA-15 Supports — ***Shyamal ROY***

Paper 582bu: One Preparation Method of High-Aluminium-Content Sulfated Zirconia: The Influence of Aluminum Contents and Washing on the Structural Morphology, Acidity and Reactivity — ***Zhiming Ma****, Li Shi*

Paper 582bv: Nature and Consequences of Al-Al Interactions in SSZ-13 Zeolite — ***Hui Li****, Tae Bum Lee, Sichi LI, Anthony DeBellis, Subramanian Prasad, Imke Britta Mueller, Ahmad Moini, William F. Schneider*

Paper 582bw: Effect of Acid Site Proximity on Acid Strength and Reaction Rates in Zeolites — ***Steven V. Nystrom Jr.****, John R. Di Iorio, Rajamani Gounder, David Hibbitts*

Paper 582bx: Aqueous One-Pot Synthesis of Pd-Based Core@Shell Catalysts with Tunable Core and Shell Sizes — ***Chang Yup Seo****, Mohit Nahata, Galen B. Fisher, Johannes W. Schwank*

Paper 582by: Application of Alginate Film-Supported Nano-Silver Catalyst — ***Supriya .****, Jayanta Kumar Basu, Sonali Sengupta*

Paper 582bz: Reduction Kinetics of Hercynite Materials Using Isoconversional Methods for Solar Thermochemical H_2O Splitting — ***Ibraheam Al-Shankiti****, Hicham Idriss, Alan W. Weimer*

Paper 582ca: Versatile Surface Modifications for Functionalization of Fibers — ***Christy Wheeler West****, Kevin N. West, T. Grant Glover, Mack Bozman, Charles Moran*

Paper 582cv: Synthesis of Pd Nanocatalysts on the Multilayered Polyelectrolyte Film in a Gas-Liquid-Solid Microreactor for Nitrobenzene Hydrogenation — ***Jian Liu****, Xun Zhu, Qiang Liao, Rong Chen, Dingding Ye, Biao Zhang*

■ HETEROGENEOUS CATALYSIS (SMALL MOLECULE)

Paper 582cb: Extinction Strain Rate Sensitivity and Calculation for Large Mechanisms — ***Alan Long****, Paul Barton, William H. Green*

Paper 582cc: Catalytic Performance and Regeneration of Gallium- and Platinum-Promoted ZSM-5 Zeolite Catalysts in Ethane Aromatization — ***Xinwei Bai****, Anupam Samanta, Brandon Robinson, Huali Wang, John Hu*

Paper 582cd: Catalytic Decomposition of Methane into CO_x Free Hydrogen and Carbon Nanotubes over Mono and Bimetallic Ni, Fe, Co Catalysts — ***Deepa Ayillath Kutteri****, I-Wen Wang, Anupam Samanta, Huali Wang, John Hu*

Paper 582ce: Novel Approach of NO_x Removal from Exhaust Gas — *Yu Liu,* ***Tan Huang****, Jong-Min Lee*

Paper 582cf: CO_2-Utilizing Chemical-Looping Reforming with the Phase Merge of Fe_2O_3–NiO to $NiFe_2O_4$ in a Perovskite Shell — *Hyun Suk Lim,* ***Dohyung Kang****, Jae W. Lee*

Paper 582cg: The Effect of CO_2 on FTS over FBR System for Applications in GTL-FPSO Process — *Gi Hoon Hong, Young Su Noh, Ji In Park, Seol A. Shin,* ***Dong Ju Moon***

Paper 582ch: Hydrogen Production by Steam Reforming of Methane over Nickel-Based Catalysts Supported on the Alumina Mixed with SiC — *Young Su Noh, Gi Hoon Hong, Ji In Park, Seol A. Shin,* ***Dong Ju Moon***

Paper 582ci: Calcium and Manganese-Doped Lanthanum Iron Perovskite Oxides as Candidate Redox Materials for CO_2 Reduction to CO — ***Bryan J. Hare****, Debtanu Maiti, Adela E. Ramos, Venkat R. Bhethanabotla, John N. Kuhn*

Paper 582ck: Low-Temperature Catalytic Gasification of Particulate Waste for In-Situ Resource Utilization — ***Uchechukwu Obiako****, Eric M. Lange, Samuel Sanya, Jorge E. Gatica*

Paper 582cl: Fast Cycling to Achieve High NO_x Conversion in Exhaust: Role of Ceria — ***Zhiyu Zhou****, Michael Harold, Dan Luss*

Paper 582cm: Cobalt Supported on Hydrothermally Synthesised Carbon Spheres for Fischer-Tropsch Synthesis — ***Mahluli Moyo****, Haifeng Xiong*

Paper 582cn: A User-Friendly Setup for Undergraduate Research: Combining Thermogravimetric Analysis with Micro Gas Chromatography — ***Amanda Simson****,* ***Edwin David****, Micah Fertig*

Paper 582co: Comparative Study of CO Adsorption on Zirconia Polymorphs with DRIFT and Transmission FT-IR Spectroscopy — ***Zhongyi Ma****, Litao Jia, Bo Hou, Li Debao*

Paper 582cp: Measurement of Raman Spectra During Thermal Oxidation of Hydrocarbon Fuels — ***Andrew L. Wagner****, Andrew Carpenter, Paul E. Yelvington*

Paper 582cq: Effects of Controlled Crystalline Plane of Hydroxyapatite on Methane Conversion Reactions — *Su Cheun Oh, Dongxia Liu*

Paper 582cr: Catalysis Research Gas Analysis Using Micro GC Fusion — ***Christina Heacox***

Paper 582cs: Investigation of the Effect of Reducing Agents (Syngas, H_2 and CO) on Catalyst Deactivation During Low-Pressure Fischer-Tropsch Synthesis — ***Joshua Gorimbo****, Adolph Muleja, Xiaojun Lu, Yali Yao, Diane Hildebrandt, David Glasser*

Paper 582ct: Integration of Random Pore Model & Langmuir-Hinshelwood Kinetics to Study High-Temperature Coal Gasification — ***Krishna Rajendren****, Sarma Pisupati*

Paper 582cu: Coal Char Gasification in CO_2 and CO Atmosphere: Effect of Pressure on the Inhibiting Behavior of CO — *Vijayaragavan Krishnamoorthy,* ***Sarma Pisupati***

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(583) Poster Session: Environmental Division
Wednesday, Nov 1, 3:15 PM
MCC, Exhibit Hall B

Debalina Sengupta, Chair
V. Faye McNeill, Co-Chair

Sponsored by: Environmental Division

Paper 583b: The CO_2, NO_x, SO_x Adsorbing Capacity of Polyaniline-Based Composite Materials — *Huang Jia, Gao Lin, Liyuan Shan, Binglu Meng, Delong Xu, Youhai Yu,* ***Yong Min***

Paper 583c: Performance of Ion-Selective Electrodes (ISE) on Wastewaters from Power Plants — ***Kyle McGaughy****, Jay Wilhelm, M. Toufiq Reza*

Paper 583d: Cesium Removal by Immobilization of Potassium Copper Hexacyanoferrate in a Cellulose-Hydrogel Network — *Yonghwan Kim,* ***Yun Kon Kim****, Sungjun Kim, David Harbottle, Jae W. Lee*

Paper 583e: Degradation Behavior of Palm Oil Mill Effluent in Fenton Oxidation — ***Disni Gamaralalage****, Osamu Sawai, Teppei Nunoura*

Paper 583f: Removal of Bromine from Tetrabromobisphenol A in an Amine Aqueous Solution Under Hydrothermal Conditions — ***Yuta Kimura****, Junichi Sakabe, Toshitaka Funazukuri*

Paper 583g: Iron/Palladium Nanoparticle-Functionalized Membrane System for Chlorinated Contaminates Treatment — ***Hongyi Wan****, Nicolas Briot, Anthony Saad, Lindell Ormsbee, Dibakar Bhattacharyya*

Paper 583h: Development of Challenging Technology on Combustion Hindrances in Commercial Solid-Refuse Fuel Combustion Facility — ***Doyeon Lee****, Jae Hyeok Park, Seung-Yong Lee, Jaehyeon Park, Dowon Shun, Dal-Hee Bae*

Paper 583i: Degradation of Organic Contaminants from Wastewater by Photocatalytic Methods via TiO2 Thin Films and Simultaneous Production of Hydrogen: Preliminary Results — ***Sunil Rawal****, Njideka H. Okoye, Satish Mahajan, Pedro E. Arce*

Paper 583j: $Li_4Ti_5O_{12}$ Pouch Cell Battery System for Selective Lithium Recovery from Aqueous Resources — ***Chosel P. Lawagon****, Grace M. Nisola, Wook-Jin Chung*

Paper 583k: Sequential Use of UV/H_2O_2—(PSF/TiO_2/MWCNT) Mixed-Matrix Membranes for Dye Removal in Water Purification: Membrane Permeation, Fouling, Rejection, and Decolorization — ***Negin Koutahzadeh****, Milad R. Esfahani, Pedro E. Arce*

Paper 583l: First-Principles Assessment of Carbon Dioxide (CO_2) Capture Mechanisms in Aqueous Piperazine (PZ) Solution — ***Haley Stowe****, Gyeong Hwang*

Paper 583m: Nascent Soot Formation by Agglomeration and Surface Growth — ***Georgios A. Kelesidis****, Eirini Goudeli, Sotiris E. Pratsinis*

Paper 583n: N-Isopropylacrylamide (NIPAAm)-Based Thermal-Responsive Composites for Polychlorinated Biphenyls (PCBs) Removal from Water — ***Shuo Tang****, Thomas Dziubla, J. Zach Hilt*

Paper 583o: Biodegradation of Oligotrophic Waters Contaminated with Chloroacetanilides Using Bacterial Mesophylic Consortiums — ***Boris Guzman Martinez Sr.****, Jose J. Castro-Arellano, Enrique Rico*

Paper 583p: Colloidal Transport in a Microfluidic Porous Medium with Surface Charge Heterogeneity — ***Yang Guo****, Keith B. Neeves, Ning Wu, Jae Kyoung Cho, Xiaolong Yin, Kenton Rod, Wooyong Um, Jaehun Chun*

Paper 583q: Magnetic Nanocomposite Materials as Reusable Adsorbents for Chlorinated Organics in Contaminated Water — ***Angela Gutierrez****, Thomas Dziubla, James Z. Hilt*

Paper 583r: Colloidal Transport in a Surface-Charge Heterogeneous Microfluidic Porous Medium — ***Yang Guo****, Keith B. Neeves, Ning Wu*

Paper 583s: Elimination of Organic Compounds in Liquid Effluents Using Mexican Natural Zeolite Impregnated with Fe by the Photo-Fenton Process — *Jose Domenzain-Gonzalez,* ***Luis A. Galicia-Luna****, Jose J. Castro-Arellano*

Paper 583t: Pretreatment of Solid Wastes from Vegetable Processing for Biofuel Production — ***Emmanuel Revellame****, William Holmes, Dhan Lord Fortela, Donald Blue*

Paper 583v: Degradation of Organic Contaminants from Wastewater by Photocatalytic Methods via TiO2 Thin Films and Simultaneous Production of Hydrogen: Preliminary Results —

Paper 583w: Determining the Structure of Hydrothermal Char and Its Effect on Adsorption Capacity — ***Avery Brown****, Brendan Mckeogh, N. Aaron Deskins, Michael T. Timko*

Paper 583x: Ceramic Tubular MOF Hybrid Membrane Fabricated Through In-Situ Layer-by-Layer Self-Assembly for Nanofiltration — ***Rong Zhang****, Dejun LIU, Jing Fu, Ning Ma, Tian Luo*

Paper 583y: Separation of Oil-in-Water (O/W) Emulsion Using Commercial Microfiltration Membranes and Sand Filters — ***Kean Wang****, Yang Yang*

Paper 583z: Study of Microplastics in Fresh Water Environment — *Jingyi Li, Huihui Liu,* ***Chen J. Paul***

Paper 583aa: Adsorption and Kinetic Studies of Using Sewage Sludge Ash in the Removal of Chemical Oxygen Demand from Domestic Wastewater, with Artificial Intelligence Approach — *Rasha A. SaryEl-deen, Ahmed S. Mahmoud, M. S. Mahmoud,* ***Mohamed K. Mostafa***

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(584) Poster Session: Fuels and Petrochemicals Division
Wednesday, Nov 1, 3:15 PM
MCC, Exhibit Hall B

Saadet Ulas Acikgoz, Chair

Sponsored by:
Fuels and Petrochemicals Division

Paper 584a: The Structural Characteristics of Oil Shale Kerogens Changed with Their Humic Degree — *Qian Wang, Qing Liu, Fan Yang, Yucui Hou,* ***Weize Wu***

Paper 584b: Database for Petroleum Fractions Components Identification — ***Lorena L. Farah****, Rita M. B. Alves*

Paper 584c: Development and Application of a Fuel Property Database for Mono-Alcohols as Fuel Blend Components for Spark Ignition Engines — ***Saeid Aghahossein Shirazi****, Kenneth F. Reardon*

Paper 584d: Microstructure of Asphaltenes in Solvent Blends Investigated by Viscosimetry — ***Weiyi Kong***

Paper 584e: Study on Crude Oil Extraction Method from Sludge Including Oil — ***Tadashi Sano****, Masatomo Watanabe, Hideaki Kurokawa, Kei Hayashida, Hisashi Isogami, Yojiro Hayashi*

Paper 584f: Insight into Coal Structure Based on Benzene Carboxylic Acids from Coal via Oxidation — *Fan Yang, Yucui Hou, Muge Niu, Shuhang Ren,* ***Weize Wu***

Paper 584g: Catalytic Oxidation of Biomass to Formic Acid Using $H_5PV_2Mo_{10}O_{40}$: Increasing Formic Acid Selectivity by Addition of Alcohols — *Ting Lu, Yucui Hou, Muge Niu, Shuhang Ren, Zengqi Lin,* ***Weize Wu***

Paper 584h: Production of Carboxylic Acids from Lignite with Two-Stage Alkali-O_2 Oxidation — ***Yucui Hou***

Paper 584i: Methane Production from Crude Solid Residue: A Minimal Organic Waste Strategy — ***Aditi David****, Saurabh Dhiman, Glenn Johnson, Rajesh Sani*

Paper 584j: Production of Carboxylic Acids from Lignite with Two-Stage Alkali-Oxygen Oxidation — ***Yucui Hou****, Wenbin Li, Fan Yang, Shuhang Ren, Weize Wu*

Paper 584k: CFD Modeling of Immiscible Liquid-Liquid Flow in a Large-Scale Crude Oil Storage Tank Equipped with Side-Entering Mixers — *Reynaldo Fonseca Sr., Diener Volpin Ribeiro Fontoura, Nicolas Spogis,* ***José Roberto Nunhez***

Paper 584l: Reaction Kinetics of 1-Methylnaphthalene Hydrocracking over Metal/Beta Catalyst to BTX — *Tao Wu,* ***Sheng-Li Chen****, Guimei Yuan, Jie Xu, Ling-xiang Huang, Ying-qian Cao*

Paper 584m: CO_2 Micro Foam and Its Application in Enhanced Oil Recovery — ***Shuangxing Liu***

Paper 584n: Catalytic Oxygen Oxidation of Lignite to Carboxylic Acids in Aqueous Solution — *Fan Yang, Yucui Hou, Muge Niu, Shuhang Ren,* ***Weize Wu***

Paper 584o: Kinetic Modelling of the Combustion of Aliphatic Hydrocarbons — ***Okoh Elechi***

Paper 584p: Predicting the Properties of Petroleum Blends — *Hessa AlMulla,* ***Tareq Albahri***

Paper 584q: On-Sun Demonstration of Hydrogen Production via Solar Thermochemical Water Splitting — ***Samantha L. Millican****, Amanda Hoskins, Caitlin Czernik, Mark Wallace, Ibraheam Al-Shankiti, Judy Netter, Charles B. Musgrave, Alan W. Weimer*

Paper 584r: Optimal Aspect Ratio and Recirculation Rate for LNG Storage Tanks in a Regasification Terminal — ***Mohd S. Khan****, Surya Effendy, S. Farooq, Iftekar Karimi*

Paper 584s: Study on Solidification Rate During the Phase Transformation Process of Pure Ethanol in the Annular Channel — ***Wei Qiu****, Wensheng Lin, Siyue Zhao*

Paper 584t: Update: Gas Production from the SCOOP — ***Richard L. Long Jr.***

Paper 584u: The Relationship Between Olefin Hydrogenation and Octane Number Loss in FCC Gasoline Hydrodesulfurization — *Lixia Dong,* ***Liang Zhao****, Kaiwei Luo, Yuhao Zhang, Jinsen Gao, Chunming Xu*

Paper 584w: Inherent Safety Assessment in Natural Gas Liquefaction Process — ***Dae-Hyun Kim****, Hye-Ri Gye, Chul-Jin Lee*

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(585) Poster Session: General Topics on Chemical Engineering II
Wednesday, Nov 1, 3:15 PM
MCC, Exhibit Hall B

Sipho C. Ndlela, Chair
David Reeder, Co-Chair

Sponsored by: Miscellaneous

Paper 585a: Multiscale Characterization and CFD Simulation of W/O Emulsions — ***Juan Pablo Gallo-Molina****,* ***Nicolas Ratkovich****,* ***Oscar Alvarez***

Paper 585b: The Use of Gas Pressure Profiles to Enhance Blending in Conical Hoppers and Cone-in-Cone Blenders — ***Kerry Johanson***

Paper 585c: Mixing and Interaction of Two Reactive Droplets in a Powder Bed — ***Ting-Yu Cheng****, Pankaj Doshi, Ying-Chih Liao*

Paper 585d: Removal of Color by Eletrocoagulation Method: Preliminary Results in Textile Dyes — *Perez Criado Sergio,* ***Vinicyus R. Wiggers****, Savio L. Bertoli, Gonçalves Marcel Jefferson, Tavares Lorena Benathar Ballod*

■ **SUSTAINABILITY AND ENERGY EFFICIENCY**

Paper 585e: A Win-Win Strategy for Chemical Plant Shutdown: Integrating Economic and Environmental Objectives — ***Sijie Ge***, *Sujing Wang, Qiang Xu, Thomas Ho*

Paper 585g: Three-Dimensional Photovoltaic Microyarns with Efficient Optoelectronic Performance and Enhanced Exciton-Hole Pair Separation — ***Jasim Uddin***, *Jared Jaksik, Erin M. Durke*

Paper 585h: Kinetic Study of Thermal Degradation of 2-Amino-2-Methyl-1-Propanol to Cyclic 4,4-Dimethyl-1,3-Oxazolidin-2-One — ***Naser S. Matin***, *Jesse G. Thompson, Femke M. Onneweer, Kunlei Liu*

Paper 585i: Energy-Integrated Natural Gas Liquid Recovery Process by Introducing Vapor-Recompressed Internally Driven Reboiler — ***Bandaru Kiran***

■ **AMMONIA**

Paper 585j: Developing a Modern Renewable Fuel Standard for Gasoline in Ontario: Ammonia (NH_3) as a Potential Transportation Solution for Ontario — ***Greg Vezina***

Paper 585k: Block Copolymer–Derived Nanoporous Carbon Membranes for High-Throughput Gas Separation — ***Kumar Varoon Agrawal***, *Mostapha Dakhchoune*

Paper 585l: Deep Decarbonization of the World's Largest Industry: Ammonia's Role as Low-Cost Energy Carrier and Storage Medium in Integrated, Optimized, Continental Systems for Total Energy Supply — ***William C. Leighty***

Paper 585m: Achievements of High Capacity and Low Energy Consumption with Ammonia Converter Replacement — ***Alvina Elysia Dharmawangsa***, *Ahmad Mardiani*

Paper 585n: Transition Metal Halides for Solid-State Ammonia Storage: The CoX_2-NH_3 System (X=Cl-I) — ***Jawza Alnawmasi***

Paper 585o: Flowsheet Safety and Techno-Economic Analysis of Ammonia and Urea Production Route — ***Ahmed AlNouss***, *Fadwa T. Eljack*

Paper 585p: Adaptive Test Bed for Anhydrous Ammonia-Based Energy Systems — ***Matthew Kern***

Paper 585q: Government of Canada Clean Fuel Standard Discussion Paper: Ammonia (NH_3) as a Carbon-Free Fuel — ***Greg Vezina***

Paper 585r: Economic Analysis of Ammonia Production Using Renewable Energy — ***Douglas Tiffany***

Paper 585s: Ammonia Renewable Energy Systems at Continental Scale: Alternative to Electricity for Transmission, Storage, and Integration for Deep Decarbonization of World's Largest Industry — ***William Leighty***

Paper 585t: Ammonia Storage in Metal-Organic Framework Materials — ***Martin Jones***, *Adrian Porch, Michael Barter, Ross Forgan*

■ **DESIGN**

Paper 585u: Optimal Design Strategy of an Aerated Stirred-Tank Reactor Using Computational Fluid Dynamics and Bayesian Multi-Objective Optimization Combined Method — ***Seongeon Park***, *Minjun Kim, Jonggeol Na, Jinjoo An, Chonghun Han*

Paper 585w: Chemical Product Design Using a Novel Computer-Aided Model-Based Tool — ***Sawitree Kalakul***, *Mario Richard Eden, Rafiqul Gani*

Paper 585x: Accelerated Process Innovation Through Hybrid Computational Modeling — *Harshavardhan Babu Namburi, Aashish Goyal, Tukaram Suryawanshi,* ***Mothivel Mummudi***

Paper 585y: Single- and Multi-Objective Optimizations Using Parallelized Process Simulators — ***Trevor Rice***, *Aaron Herrick, Mingder Lu*

Paper 585z: Liquid-Liquid Extraction in Stratified Flow in a Wavy-Wall Microchannel — ***Anil Vir***, *V. Leela Vinodhan, S. Pushpavanam*

Paper 585aa: PROCADF: A Tool for Generating Sustainable Hybrid Process Flowsheets — ***Anjan Kumar Tula***, *Mario Richard Eden, Rafiqul Gani*

■ **BIOMATERIALS & BIOTECHNOLOGY**

Paper 585ac: Bio-Ionic Liquid-Functionalized Biomaterial — ***Iman Noshadi***

Paper 585ad: Effect of Electrical Stimulation on Nerve Cells as a Function of Hydrogel Stiffness and Electrical Conductivity with a Custom-Designed Device — ***Mozhdeh Imaninezhad***, *Kristin Kalinowski, Reetom Bera, Fenglian Xu, Silviya Petrova Zustiak*

Paper 585ae: IVF Modeling, Optimal Control, and Customized Drug Treatment: Results of First Clinical Trial — ***Urmila M. Diwekar***, *Kirti Yenkie, Vibha Bhalerao*

Paper 585ag: Tissue Patterning by Spatially Defined Addressable Microfluidic Delivery of Differentiated Growth Factors — ***Long Quang Pham***, *David Chege, Timothy Dijamco, Nhat-Anh N. Tong, Sagnik Basuray, Roman Voronov*

Paper 585ai: Multiscale Modeling of Drug Transport Through Human Skin Stratum Corneum — ***Kishore Gajula***, *Rakesh Gupta, Dwadasi Balarama Sridhar, Beena Rai*

Paper 585ak: Jet Hydrodynamics in Needle-Free Injection — ***Jeremy Marston***, *Jonathan Simmons*

Paper 585al: Integrated Design of Sulfur Host Materials to Enhance the Performance of Li-Sulfur Batteries — ***Sarish Rehman,*** *Kishwar Khan*

Paper 585am: Porous and Chemically Functional Polymeric Hydrogel Microspheres for Improved Biomacromolecular Conjugation — ***Eric Liu***, *Sukwon Jung, Chang-Hyung Choi, Hyunmin Yi*

Paper 585an: Engineered CRISPR/Cas9 System for Multiplex Genome Engineering of Industrial Yeast Strains — ***Jiazhang Lian***, *Sumeng Hu, Huimin Zhao*

Paper 585ao: Accelerating Build and Test of Microbial Libraries via Integration of Synthetic Biology, Robotic Automation and Mass Spectrometry — ***Tong Si***, *Wilfred A. van der Donk, Jonathan V. Sweedler, Huimin Zhao*

Paper 585ap: Cell-Free Synthetic Biology: An Emerging Strategy to Revolutionize the Biomedical Industry — ***Yuan Lu***

Paper 585aq: Encapsulation, Protection and Programmed Release of Active Ingredients from Silicone Gel Particles for Topical Applications — ***C. Wyatt Shields IV***, *John White, Erica Osta, Nickolas Kirby, Jerishma Patel, Shashank Rajkumar, Stefan Zauscher*

Paper 585ar: Long-Term Adaptive Evolution of Amberless *Escherichia coli* Strains Reveals Selective Mutations in Translation Machinery — ***Aditya M. Kunjapur***, *Timothy M. Wannier, Daniel Rice, Michael McDonald, Michael M. Desai, George M. Church*

Paper 585as: Award Session: Laser-Activated Sealants for Skin Tissue Repair — ***Russell Urie***, *Deepanjan Ghosh, Mitzi Thelakkaden, Chengchen Guo, Jeff Yarger, Jacquelyn Kilbourne, Kaushal Rege*

Paper 585at: Non-Natural Redox Cofactor-Wired Metabolic Circuits — ***Zongbao Zhao***

■ **CATALYSIS**

Paper 585au: Evaluation of Forming and Mechanical Properties of Catalysts Base Zeolite — ***Karla D. Guerrero G.***, *Julio C. Vargas*

Paper 585av: Designing Pellet Shapes for the Dynamic Catalytic Methanation in Fixed-Bed Reactors Using Particle-Resolved CFD Simulations — ***Gregor D, Wehinger***, *Thomas Turek*

Paper 585ay: Interplay Between Dopant and Oxygen Vacancy in a TiO2 Support Enhances the Oxygen Reduction Reaction — ***Bing Joe Hwang***, *Wei-Nien Su, Men-Che Tsai, Bing-Jen Hsieh*

Paper 585az: Insights into the Isobutane Alkylation with Butene Catalyzed by the Combination of SO_3H-Functionalized Ionic Liquids and Sulfuric Acid — ***Weizhen Sun***, *Wenxiu Xie, Weizhong Zheng*

Paper 585ba: Alkylation of Isobutane and Butene Using Mixed Acid as Catalyst — ***Liantang Li***, *Jisong Zhang, Kai Wang, Luo Guangsheng*

Paper 585bb: Base-Free Aerobic Oxidation of 5-Hydroxymethylfurfural to 2, 5-Furandicarboxylic Acid over Nanoscale Pt Catalysts Prepared by Atomic Layer Deposition — ***Jie Fu***, *Hao Chen, Jinshan Shen, Xiuyang Lu*

Paper 585bc: Strategies for Improving Active Chemistry, Mitigation of Coke Formation and Sustaining Selectivity to Benzene in the Catalytic Aromatization of Methane — ***Sheima J. Khatib***, *Mustafizur Rahman, Apoorva Sridhar, James Tata, Leah Harper, Eva Osoro*

Paper 585bd: Preparation of the Graphite-Phase Carbonic Nitrogen ($g\text{-}C_3N_4$) for Photocatalytically Reducing CO_2 — ***Xiaohong Yin***, *Xiao Shao*

Paper 585be: The Synthesization of SAPO-11 and Its Catalytic Performance for the Alkylation of Naphthalene — ***Wei Zhang Sr.***, *Debao Li, Litao Jia, Bo Hou*

Paper 585bg: Role of Active Sites in the CO_2 and Steam Gasification of Model RDF Char — ***Sireesha Aluri***, *Pradeep K. Agrawal, Carsten Sievers, John D. Muzzy, Derrick W. Flick, Brien Stears*

Paper 585bh: Computer-Generated Microkinetic Mechanisms: Applications for Catalytic Combustion of Methane on Pt — ***C. Franklin Goldsmith***, *Richard H. West*

Paper 585bi: N-Doped Carbon Aerogel-Supported Cobalt Catalysts by Supercritical Deposition for Oxygen Reduction Reaction — ***Secil Unsal***, *Selmi Erim Bozbag, Can Erkey*

Paper 585bk: Optimizing Acid-Stable Metal Oxides for Oxygen Evolution Reaction — ***Michal Bajdich***

Paper 585bm: Metal Nanoparticles Encapsulated in Melamine Dendrons Supported on MCM-41 and SBA-15 — ***Daniel Shantz***, *Yueyun Lou, Aibolat Koishybay*

Paper 585bn: An Improved Catalyst Deactivation Protocol on Commercial FCC Catalysts for Higher Conversion of Residual Feedstock — ***Balasubramanian Vaithilingam,*** *Gnana Pragasam Singaravel, Abdul Majed Al Katheeri, Stephane M., Mikael Berthod*

Paper 585bo: Computational Design of Near-Surface Alloyed Oxide for Water Splitting — ***Liang Zhang***, *Aleksandra Vojvodic*

Paper 585bp: Global Kinetic Modelling and Reactor Analysis of Lean NO_x Traps Catalysts (LNT) — ***Nishithan Balaji***, *Preeti Aghalayam, Niket S. Kaisare*

Paper 585bq: Issues in Primary Reformer Catalyst Replacement After 16 Years of Operation — ***Arshad Naveed***, *Muhammad Waqas Quraishi, Muhammad Majid Latif*

Paper 585bs: Photocatalytical Degradation of Congo Red (CR) Dye by Nano Titanium Dioxide–Coated Glass Bead Under UV Light — ***Asad Khan***, *Khurram Tahir, Zaki Ahmad*

Paper 585bt: Highly Efficient Photocatalytic Degradation of Organic Pollutants by TiO_2-PDMS Composite Sponge — ***Renae Hickman***, *Sanchari Chowdhury*

Paper 585bu: Kinetics of the Water-Gas Shift over a Cu-Based Catalyst for Pyrolysis Vapor Upgrading — ***Ross Houston***, *Nourredine Aboulmoumine, Nicole Labbé*

Paper 585bv: Superwetting Electrodes for Gas-Involved Electrocatalysis — ***Xiaoming Sun***

Paper 585bw: Anodic Aluminum Oxide–Supported Cu-Zn Catalyst for Steam Reforming of Methanol — ***Dong Hyun Kim***, *Jung Hyeon Kim*

(586) Poster Session: Process Development
Wednesday, Nov 1, 3:15 PM
MCC, Exhibit Hall B

Joe Schroer, Chair
Liwen Chen, Co-Chair

Sponsored by:
Process Development Division

■ **PROCESS & SEPARATIONS DESIGN**

Paper 586a: Characterization and Evaluation of Zero-Length Covalent Crosslinking Strategies for DNA-Based Applications — ***Malithi Wickramathilaka***

Paper 586b: Adsorption Desulfurization Performance of B_2O_3-Modified Ag-CeO_x/TiO_2-SiO_2 and Adsorption Diffusion Study — ***Meiqin Zheng***, *Xiaohui Chen,* ***Hui Hu***

Paper 586c: Experimental Vapor-Liquid Equilibrium Data for the Ternary Mixture (Methane + Propane + Methylbenzene) at Conditions Relevant to the LNG Scrub Column — *Fernando Perez, Saif Al-Ghafri,* ***Eric F. May***

Paper 307e: Effect of Non-Ideal Behavior on the Energy Minimum Design of Highly Integrated Reaction and Separation Processes — *Laura-Selin Cici, Georg Fieg,* ***Torben Egger***

■ **OPTIMIZATION & CONTROL**

Paper 586d: Reactive Dividing-Wall Column: Experimental and Simulative Studies About Process Control and Dynamic Behaviour — ***Lisa Egger***, *Georg Fieg*

Paper 586e: A Thermodynamic-Based Modeling and Analysis Approach for Mechanical Energy Recovery — ***Aida Amini Rankouhi***, *Yinlun Huang*

Paper 586f: Influence of Transport Properties and Correlations Between Properties in Process Modeling — *Pia Herrmann, Kevin Busch,* ***Karsten Müller***

Paper 586g: Life-Cycle Optimization of Topside Process Design for Offshore Platform — ***Ziehyun Kim***, *Soojin Kwon, Yeonju Shin, Yeonpyeong Jo, Seungwook Cho, Sungwon Hwang*

(587) Poster Session: Sustainability and Sustainable Biorefineries
Wednesday, Nov 1, 3:15 PM
MCC, Exhibit Hall B

Nastassja Lewinski, Chair
Cory Jensen, Co-Chair
Ashley M. Pennington, Co-Chair

Sponsored by: General

Paper 587a: Rapid Estimation of Life-Cycle Inventories — ***Raymond L. Smith***, *David E. Meyer, Gerardo J. Ruiz-Mercado, Vinit K. Mittal, Michael A. Gonzalez, John P. Abraham, William M. Barrett, Paul M. Randall*

Paper 587b: Aspects of Sustainable Production of Palm Oil in the Municipality of Teapa in Tabasco, Mexico: Evaluating the Current and Future Use of Palm Oil — ***Bethany Klemetsrud***, *Carlos García, Cesar J. Vazquez-Navarrete, Jessie Knowlton, Amarella Eastmond, Erin Pischke, Ena Mata Zayas*

Paper 587c: Harvesting and Extraction Technologies Contributing to Algae Biofuel Environmental Viability: Life-Cycle Analysis of NAABB-Developed Novel Technologies — ***Rui Shi,*** *Robert Handler, David R. Shonnard*

Paper 587d: Comparative Techno-Economic Analysis of Algal Biofuel Production via Hydrothermal Liquefaction: One Stage Versus Two Stages — ***Xiangyu Gu***, *Shulin Chen, Liang Yu*

Paper 587e: Economic and Environmental Assessment for the Production of Propylene Glycol from Biodiesel Glycerol — *Andres Gonzalez-Garay, Maria Gonzalez-Miquel,* ***Gonzalo Guillén-Gosálbez***

Paper 587f: More Than Ethanol: A Techno-Economic Analysis of Corn Stover-Ethanol Biorefinery Integrated with Hydrothermal Liquefaction Process to Convert Lignin into Biochemicals — ***Denis Bbosa***, *Mark Mba Wright*

Paper 587g: A Mixed-Integer Programming Model for Municipal Waste Management and Landfill Gas-to-Energy Systems — ***Vicente Rico-Ramirez***, *Jaime Garibay-Rodriguez, Salvador Hernandez-Castro, Jose E. Botello-Alvarez*

Paper 587h: Techno-Economic Analysis of Integrated Solid Oxide Fuel Cell–Gas Turbine–Organic Rankine Cycle Powered by Seaweed Biogas — ***Ivannie Effendi***, *Peyman Fasahati, J. Jay Liu*

Paper 587i: Membrane Pervaporation in a Fast-Pyrolysis Biorefinery — ***John P. Stanford***, *Preston A. Gable, Patrick H. Hall, Marjorie R. Rover, Ryan G. Smith, Robert Brown*

Paper 587j: Photocatalytic Reforming of Biomass for Hydrogen Production — ***R. M. Ripken***, *V. J. H. W. de Boer, J. G. E. Gardeniers, S. Le Gac*

Paper 587k: Experimental Analysis of Catalytic Gasification of Waste — ***Samuel Sanya***, *Uchechukwu Obiako*

Paper 587l: Investigation of Closed-Loop Bioponic Irrigation Systems for Urban Agriculture — *David R. Shonnard,* ***Anthony Jones***

Paper 587m: A Mechanistic Model for the Product Distribution of Fast Pyrolysis of High-Density Polyethylene Waste — ***Ulises R. Gracida-Alvarez***, *Dillon Gronseth, Mary Kate Mitchell, Julio C. Sacramento-Rivero, David R. Shonnard*

Paper 587n: A Model-Based Approach for Sustainability Assessment of Biomethane from Anaerobic Digestion of Food Waste and Manure Mixtures — ***Sharath Ankathi***, *David R. Shonnard, Natalia Parra-Alvarez*

Paper 587o: Efficient Saccharification of Softwoods by an Integrated Thermochemical and Biological Process — *Md. Anwar Hossain, Thanh Khoa Phung, Sarttrawut Tulaphol, Teerawit Prasomsri, Noppadon Sathitsuksano,* ***Mohammad Shahinur Rahaman***

Paper 587p: Single-Objective Versus Multi-Objective Optimization of Integrated Fermentation and In-Situ Product Recovery Based on Time-Dependent Fermentation Models — ***Kwabena Darkwah***, *Jeffrey Seay, Barbara L. Knutson*

Paper 587q: Enzyme Cocktail Design of β-Agarase Enzymes for Complete Hydrolysis of Agarose in Ionic Liquid-Pretreated *Gelidium amansii* — *Teklebrahan G. K. Weldemhret,* ***Grace M. Nisola***, *Kris Niño G. Valdehuesa, Wook-Jin Chung*

Paper 587r: Development of Bottom-Up Life-Cycle Inventory Methods for Chemical Reaction Systems — ***William M. Barrett***, *Raymond L. Smith, Gerardo J. Ruiz-Mercado, David Meyer, Michael A. Gonzalez, John P. Abraham*

Paper 587s: Simultaneous Production of Biogas and Hydrogen using Microbial Electrolysis Cell Integrated with Anaerobic Digester— ***Samsudeen Naina***, *Jagannadh Satyavolu*

(588) Active Colloidal Systems
Wednesday, Nov 1, 3:15 PM
MCC, M100A

Christopher L. Wirth, Chair
Ning Wu, Co-Chair
Daphne Klotsa, Co-Chair

Sponsored by: Interfacial Phenomena

3:15 Paper 588a: Out-of-Equilibrium Phase Behavior of Dielectric/Paramagnetic Nanoparticle Suspensions in Toggled Electric/Magnetic Fields — ***Zachary Sherman***, *James Swan*

3:30 Paper 588b: Investigation of the Motion of Patchy Particles at Liquid/Fluid Interfaces — ***Zohreh Jalilvand***, *Ilona Kretzschmar*

3:45 Paper 588c: Preparation and Characterization of Janus Dumbbells Nanomotors — ***Florian Guignard***, *Marco Lattuada*

4:00 Paper 588d: Magnetic Microlassos for Reversible Cargo Capture, Transport, and Release — *Tao Yang, Tonguc Onur Tasci, Keith B. Neeves, Ning Wu,* ***David W. M. Marr***

4:15 Paper 588e: Fly Larvae Mix to Increase Eating Rates — ***Olga Shishkov***, *David L. Hu*

4:30 Paper 588f: Programming the Dynamics of Active Colloids in 3D — ***JinGyun Lee***, *Stacey Wieseneck, Bhuvnesh Bharti*

4:45 Paper 588g: Tuning the Collective Behavior of Active Electrohydrodynamic Motors — ***Xingfu Yang***, *Ning Wu*

5:00 Paper 588h: Heterogeneous Active Matter Systems — ***Thomas Kolb***

5:15 Paper 588i: Directed Motion of Metallodielectric Particles by Contact Charge Electrophoresis — ***Yong Dou***, *Charles A. Cartier, Wenjie Fei, Shashank Pandey, Sepideh Razavi, Ilona Kretzschmar, Kyle J. M. Bishop*

5:30 Paper 588j: Curvature-Induced Microswarming — ***Isaac Bruss***, *Sharon C. Glotzer*

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(589) Advances in Unconventional Oil and Gas Modeling
Wednesday, Nov 1, 3:15 PM
MCC, 200C

Jared Ciferno, Chair
Rameshwar Srivastava, Co-Chair
Jason Trembly, Co-Chair
David Cercone, Co-Chair

Sponsored by:
Advances in Fossil Energy R&D

3:15 Paper 589a: Unconventional Oil and Natural Gas: Science & Technology Advancement — ***Jared Ciferno***, *David Cercone, Rameshwar Srivastava*

3:37 Paper 589b: Alternatives to Decline-Curve Models for Unconventional Reservoirs: A Case for Data-Driven Discovery of Natural Laws — ***Bharat Thakur***, *Michael Nikolaou*

3:59 Paper 589c: Production Estimation and Well Classification for Hydraulically Fractured Horizontal Wells: A Data-Driven Model-Based Approach — ***Sunit Mathur***

4:21 Paper 589d: Measurement and Modeling of Competitive Sorption of Methane/Ethane Mixtures on Marcellus Shale: Isotherms and Kinetics — ***Devang Dasani***, *Yu Wang, Theodore T. Tsotsis, Kristian Jessen*

4:43 Paper 589e: Sensitivity Study of Fracture Propagation by Foamed Fluids and Slickwater in Unconventional Reservoirs — ***Fatick Nath***, *Chongwei Xiao*

5:05 Paper 589f: Enhancing Oil Recovery from Shales: Reservoir-Specific and Economical Approach — ***Harpreet Singh***

5:27 Paper 589g: Maximizing Uniformity of Hydraulic Fracture Stimulation of Horizontal Wells Through Stress Shadow Balancing and Limited Entry Methods — ***Andrew P. Bunger***, *Cheng Cheng, Anthony P. Peirce*

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(590) Applications in Immunology and Immunotherapy
Wednesday, Nov 1, 3:15 PM
MCC, 206A/B

Steven M. Abel, Chair
Fei Wen, Co-Chair

Sponsored by:
Engineering Fundamentals in Life Science

3:15 Paper 590a: Engineering Selective Immunoglobulin E Inhibitors for Peanut Allergies — ***Peter Deak***, *Baksun Kim, Maura Vrabel, Joseph Riehm, Tanyel Kiziltepe, Basar Bilgicer*

3:33 Paper 590b: Glycan-Specific Antibody Discovery Through Designer Glycopeptide Immunization — ***Tyler D. Moeller***, *Matthew P. DeLisa*

3:51 Paper 590c: Localized Multi-Component Delivery Platform Generates Local and Systemic Anti-Tumor Immunity — ***Abhinav P. Acharya***, *Steven R. Little*

4:09 Paper 590d: Microsphere-Assisted Peptide Screening (MAPs): High-Throughput Identification of Promiscuous MHCII-Binding Peptides for T-Cell Epitope Vaccine Designs — ***Mason Smith***, *Fei Wen*

4:27 Paper 590e: Kinetic Analysis of CD3ζ and CD28 Chimeric Antigen Receptor T Cell Activation — ***Jennifer A. Rohrs***, *Dongging Zheng, Nicholas Graham, Pin Wang, Stacey D. Finley*

4:45 Paper 590f: Catch Bonds at T Cell Interfaces — ***Robert H. Pullen III***, *Steven M. Abel*

5:03 Paper 590g: Marrow-Derived & Surface-Engineered Macrophages Engorge, Accumulate, and Differentiate in Antibody-Targeted Regression of Solid Tumors — ***Dennis E. Discher***

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(591) Biomaterials for Drug Delivery II: Micellar, Polymer and Protein-Based Drug Carriers
Wednesday, Nov 1, 3:15 PM
MCC, 211B

Srivatsan Kidambi, Chair
Timothy Brenza, Co-Chair

Sponsored by: Biomaterials

3:15 Paper 591a: ATRP-Grown Protein-Polymer Conjugates Selectively Enhance Transepithelial Protein Transport — *Chad Cummings, Katherine Fein, Hironobu Murata, Rebecca Ball, Alan Russell,* ***K athryn A. Whitehead***

3:33 Paper 591b: Aptamer Micelles Targeting Cancer Cells Expressing the Chemokine Fractalkine — ***Michael A. Harris***, *Timothy R. Pearce, Thomas Pengo, Huihui Kuang, Colleen L. Forster, Efrosini Kokkoli*

3:51 Paper 591c: Non-Charged Cell-Penetrating Oligothioetheramides — ***Ngoc Phan***, *Christopher A. Alabi*

4:09 Paper 591d: Targeting, Delivery, and Immobilization of Therapeutic Factors with Native Free Radicals — ***Christopher J. Lowe***, *Keana Mirmajlesi, David I. Shreiber*

4:27 Paper 591e: Antimicrobial Peptide Amphiphile (AMPA) Medical Product Coatings for the Prevention of Nosocomial Infections — ***Josiah Smith***, *Alexis Dadelahi, Julie Nguyen, Fabio Gallazzi, John Dodam, Jeffrey Adamovicz, Roger de la Torre, Bret Ulery*

4:45 Paper 591f: Mitigating the Bioactivity Loss of Polymer-Insulin Conjugate — ***Zhiqiang Cao***, *Yang Lu*

5:03 Paper 591g: Enhancing Therapeutic Efficacy of Self-Assembling Prodrugs with Supramolecular Chemistry — ***Hao Su***, *Yuzhu Wang, Feihu Wang, Honggang Cui*

5:21 Paper 591h: Hydrogen Sulfide Donor Micelles: Synthesis, Characterization and Therapeutic Potential — ***Urara Hasegawa***, *Andre van der Vlies, Jerry J. Y. Chen, Tomoka Takatani-Nakase, Ikuhiko Nakase*

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(592) Biomaterials for Immunological Applications II: Cancer Immunotherapy and Autoimmune Disease Treatments
Wednesday, Nov 1, 3:15 PM
MCC, 211A

Bret Ulery, Chair
R. Michael Gower, Co-Chair
Peipei Zhang, Co-Chair

Sponsored by: Biomaterials

3:15 Paper 592a: Pegylation of Model Drug Carriers Enhances Uptake by Primary Human Neutrophils — ***William Kelley***, *Catherine A. Fromen, Omolola Eniola-Adefeso*

3:33 Paper 592b: "Smart" Nanoparticles for Immunotherapeutic Targeting of the Sting Pathway — *Daniel Shae, Denise Buenrostro, Alyssa Merkel, Sema Sevimli, Julie A. Sterling,* ***John Wilson***

3:51 Paper 592c: Biomaterial Nanoparticles Redistribute Therapeutic Antibodies to Lymph Node-Resident Cells to Enhance Cancer Immunotherapy via Checkpoint Inhibition — ***David Francis***, *Alex Schudel, Nathan A. Rohner, Susan N. Thomas*

4:09 Paper 592d: Engineering Nanoparticle Artificial Antigen-Presenting Cells Based on T Cell Biology Improves T Cell Enrichment and Activation for Cancer Immunotherapy — ***John Hickey***, *Fernando Vicente, Hai-Quan Mao, Jonathan Schneck*

4:27 Paper 592e: Biomaterial Scaffolds for Combined Focal Ablation and Immunotherapy to Target Disseminated Cancer — ***Francisco Pelaez***, *Stephen O'Flanagan, Qi Shao, Brandon Burbach, Tiffany Lam, John C. Bischof, Yoji Shimizu, Samira M. Azarin*

4:45 Paper 592f: Modulating the Immune Environment Within Adipose Tissue with Polymer Scaffolds — ***Kendall Murphy***, *Michael Gower*

5:03 Paper 592g: Multi-Factor Microparticle Formulation for Local Induction of Regulatory Lymphocytes and Treatment of Periodontal Disease — ***Ashlee Greene***, *Sayuri Yoshizawa, Michelle Ratay, Charles Sfeir, Steven R. Little*

5:21 Paper 592h: Multivalent Soluble Antigen Arrays Target Antigen-Presenting B Cells and Dampen Antigen-Specific Signaling to Promote Therapeutic Efficacy in Multiple Sclerosis — ***Brittany Hartwell***

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(593) Bioplastics, Biocomposites and Value-Added Uses of Biofuel Coproducts for Sustainable Manufacturing
Wednesday, Nov 1, 3:15 PM
MCC, 200B

Amar K. Mohanty, Chair
Manju Misra, Co-Chair

Sponsored by:
Forest and Plant Bioproducts Division

3:15 Introductory Remarks

3:17 Paper 593a: Novel Bio-Based Polyesters and Polycarbonates Derived from Xylochemicals — ***Joseph F. Stanzione III***, *Silvio Curia, Joseph Mauck, Alexander W. Bassett, John J. La Scala*

3:42 Paper 593b: Lightweight Biocomposite from Toughened Polyolefin and Biocarbon — *Ehsan Behazin,* ***Manju Misra***, *Amar K. Mohanty*

4:07 Paper 593c: Secondary Fermentation of Corn Ethanol Co-Products for Improved Amino Acid Qualities — ***Tanner Barnharst***, *Yanmei Zhang, Jingyu Wang, Bo Hu*

4:32 Paper 593d: Extraction of High-Value Chemicals from Ethanol Co-Products: A Feasibility Assay on Phytate Extraction with Life-Cycle and Techno-Economic Assessment — ***Cristiano Reis***, *Aravindan Rajendran, Douglas Tiffany, Bo Hu*

4:57 Concluding Remarks

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(594) Continuous Processing Technologies Applied in Drug Substance Manufacturing
Wednesday, Nov 1, 3:15 PM
MCC, 204A/B

Mark Barrett, Chair
Joe Hannon, Co-Chair

Sponsored by:
Pharmaceutical Discovery, Development and Manufacturing Forum

3:15 Paper 594a: Advanced Control Strategy Approaches for Continuous Pharmaceutical Manufacturing: The Regulatory Landscape — Thomas O'Connor

3:37 Paper 594b: Pharmacy-on-Demand: A Continuous Revolution in Pharmaceutical Manufacturing? — ***Luke Rogers***, *Ramona Achermann, Andrea Adamo, Mohsen Behnam, Rachel Beingessner, Dave Brancazio, Naomi Briggs, Jie Chen, Gregory Hammersmith, Timothy Jamison, Klavs F. Jensen, Guahua Liang, Hongkun Lin, Allan S. Myerson, Clemence Neurohr, Carter Salz, Ridade Sayin, David Snead, Dale Thomas, Nopphon Weeranoppanant, Lukas Weimann, Shin Yee Wong, Ping Zhang*

3:59 Paper 594c: Platforms for Integrated Continuous Drug Substance Design and Manufacture — ***Anna Przybyl***, *Gary Morris, Richard Wareham, Brian Glennon, Mark Barrett*

4:21 Paper 594d: Residence Time Distribution and Material Traceability for Continuous Drug Substance Processes — ***Christopher S. Polster***, *Venkata Ramana Reddy, Carla Luciani, Stephen B. Jeffery, Martin Johnson, Kevin Chinn, Hod Finkelstein*

4:43 Paper 594e: A Miniature CSTR Platform for Continuous Processing of Multiphase Systems — ***Yiming Mo***, *Klavs F. Jensen*

5:05 Paper 594f: From Grams of Drug Substance to Commercial-Scale Clinical Supply Manufacture in Less Than a Year — ***Carl Hartmann III***

5:27 Paper 594g: A Continuous and Controlled Pharmaceutical Freeze-Drying Technology for Unit Doses — ***Thomas De Beer***

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(595) Data Mining and Machine Learning in Molecular Sciences I
Wednesday, Nov 1, 3:15 PM
MCC, L100H

Johannes Hachmann, Chair
Andrew L. Ferguson, Co-Chair
Diwakar Shukla, Co-Chair

Sponsored by:
Computational Molecular Science and Engineering Forum

3:15 Paper 595a: Progress Towards Ultra-Fast Screening of Porous Sorbents for Chemical Separations — ***David S. Sholl***, *Dai Tang*

3:45 Paper 595b: Identifying New Descriptors for Gas Storage in Nanoporous Materials — ***Benjamin Bucior***, *N. Scott Bobbitt, Arun Gopalan, Randall Q. Snurr*

3:57 Paper 595c: Discovery of High-Performing MOFs via Machine Learning — ***Alauddin Ahmed***, *Donald J. Siegel*

4:09 Paper 595d: Finding Truth in Fiction: Efficiently Discovering Physical Structure-Property Relationships by Screening Unphysical Porous Materials — ***Christopher E. Wilmer***, *Alec R. Kaija*

4:21 Paper 595e: Mapping Transition Metal Chemical Space for Machine-Learning Models — ***Jon Paul Janet***, *Heather J. Kulik*

4:33 Paper 595f: Resolving 3D Structures of Metallic Nanoparticles from X-Ray Absorption Data Using Artificial Neural Network — ***Janis Timoshenko***, *Deyu Lu, Shinjae Yoo, Anatoly I. Frenkel*

4:45 Paper 595g: Identifying Descriptors for Materials Science via Genetic Programming: A Case Study for Dielectric Breakdown Strength — *Fenglin Yuan, Tim Mueller*

4:57 Paper 595h: Data-Driven Prediction of Materials Properties in an Automated Fashion — ***H. Shaun Kwak***, *Thomas J. L. Mustard, David J. Giesen, Thomas F. Hughes, Alexander Goldberg, Andrea Browning, Steve Dixon, Mathew D. Halls*

5:09 Paper 595i: Computer-Aided Design of Novel Materials with Desired Electronic and Physical Properties — ***Olexandr Isayev***

5:21 Paper 595j: Stability Prediction of Hypervalent Compounds Based on Data-Centric Modelling — ***Hans P. Lüthi***

5:33 Paper 595k: Human-Interpretable Reaction Informatics — ***Dmitry Zubarev***

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(596) Development of Processes and Products for Pharmaceuticals and Hybrid Therapeutics
Wednesday, Nov 1, 3:15 PM
MCC, 201A/B

Michael L. Hoffman, Chair
Christopher L. Burcham, Co-Chair

Sponsored by:
Pharmaceutical Discovery, Development and Manufacturing Forum

3:15 Paper 596a: Engineering Considerations for Dissolved Oxygen Sensor Response Across Silicone Membranes in 3-L Single-Use Bioreactors — ***William Tran***, *John Bowers, T. Craig Seamans*

3:36 Paper 596b: Process Development Tool to Rapidly Predict the Stability of Biopharmaceuticals — ***Sarah Hedberg***, *Yolanda Hutabarat, Jerry Heng, Jonathan Haigh, Daryl Williams*

3:57 Paper 596c: Model-Based Process Optimization for Upstream Bioreactor Production–Downstream Chromatographic Separation of CHO Cell Monoclonal Antibodies (mAb) — ***Uroš Novak***, *Drejc Kopač, Miša Cajnko, Andrej Pohar, Matic Grom, Blaž Likozar*

4:18 Paper 596d: Exploring the Multi-Minima Behavior of Organic Crystal Polymorphs at Finite Temperature — ***Eric Dybeck***, *Michael R. Shirts*

4:39 Paper 596e: Iterative Synthesis of Heteropolymers Using Organic Solvent Nanofiltration — ***Ruiyi Liu***, *Piers Gaffney, Patrizia Marchetti, Marc Schaepertoens, Ruijiao Dong, Andrew G. Livingston*

5:00 Paper 596f: Challenges in Process Development of Antibody Drug Conjugates (ADCs) — ***Vimalkumar Patel***

5:21 Paper 596g: Improved Manufacturing Process for Semi-Synthetic Calicheamicin Linker-Payload en Route to Antibody-Drug Conjugates — ***Leo J. Letendre***, *Frank W. Kotch, Amarnauth Prashad, Vimalkumar Patel, Wesley Swanson, Xi Hu, Lawrence Chen, April Xu, Sen Zhang, Stephen Freese, Eric Bortell*

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(597) Developments in Extractive Separations: Processes
Wednesday, Nov 1, 3:15 PM
MCC, M100D

Michael Trippeer, Chair
George S. Goff, Co-Chair
Megan E. Donaldson, Co-Chair

Sponsored by: Extractions

3:15 Paper 597a: Apparatus Design for Liquid-Liquid Extraction Combined with Heterogeneously Catalyzed Esterification — ***Annika Grafschafter***, ***Daniela Painer***, *Andreas Toth, Matthaeus Siebenhofer*

3:40 Paper 597b: Recovery of Both Low- and High-Molecular-Weight Lignin Fractions by Extraction with Hot Aqueous Organic Solvent Systems — ***Junhuan Ding***, *Adam S. Klett, Jordan A. Gamble, Graham W. Tindall, Mark C. Thies**

4:05 Paper 597c: Reactive Extraction of Lactic Acid with Trioctylamine/Octanol/n-Undecane — ***Nuttakul Mungma***, *Marlene Kienberger, Matthäus Siebenhofer*

4:30 Paper 597d: Using Deep Eutectic Solvents (DESs) to Extract Lignin from Black Liquor — ***Fatemeh Saadat Ghareh Bagh***, *Srimanta Ray, Jerald Lalman, Rajesh Seth, Niharendu Biswas*

TECHNICAL SESSIONS 2017

4:55 Paper 597e: Efficient and Selective Recovery of Formic Acid and Acetic Acid from Their Mixed Solutions — *Hani Zeidan,* ***Mustafa E. Marti***

5:20 Paper 597f: Simulation and Comparative Evaluation of Different Methods of Microalgal Lipid Extraction and Conversion to Biodiesel Using Aspen HYSYS — ***Geetanjali Yadav,*** *Arpit Mishra, Parthasarathi Ghosh, Ramkrishna Sen*

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(598) Drug Delivery III
Wednesday, Nov 1, 3:15 PM
MCC, 208B

Jessica Kelly, Chair

Sponsored by:
Engineering Fundamentals in Life Science

3:15 Paper 598a: Intracellular Invasion of Salmonella Drives Tumor Colonization of the Bacteria In Vitro — ***Vishnu Raman,*** *Nele Van Dessel, Owen O'Connor, Neil S. Forbes*

3:33 Paper 598b: Engineering Lipid Nanoparticles for Targeting Inflammation Site in Atherosclerosis — ***Rashi Porwal,*** *Stephen L. Hayward, Matthew Sis, Xiang-der Liu, Angelos Karagiannis, Yiannis Chatzizisis, Srivatsan Kidambi*

3:51 Paper 598c: Using Ultrasound to Enhance Tumor Cell Killing by Anti-PD1 and Doxorubicin-Loaded Particles — ***Anh-Vu Do,*** *Dongrim Seol, Phillip Tobias, James Martin, Aliasger K. Salem*

4:09 Paper 598d: Computational Study of Deformable Functionalized Nanocarrier Adhesion to the Cell Surface — ***Samaneh Farokhirad,*** *Ramakrishnan Natesan, Portonovo S. Ayyaswamy, David M. Eckmann, Ravi Radhakrishnan*

4:27 Paper 598e: Acetalated Dextran Nanoparticles for Rapid and Glucose-Responsive Insulin Delivery — ***Lisa R. Volpatti,*** *Robert Langer, Daniel Anderson*

4:45 Paper 598f: Succinylated Polyethylenimine Derivatives Enhance Gene Expression and Serum Stability In Vitro — ***Logan Warriner,*** *Joseph Duke III, Jason DeRouchey, Daniel Pack*

5:03 Paper 598g: Engineering CRISPR-Cas9 Plasmid-Loaded PLGA Nanoparticles to Repair Mutations in the TLR4 Gene in Mice — ***Ami Jo,*** *Veronica Ringel, Irving Allen, Richey M. Davis*

5:21 Paper 598h: Achieving Long-Term Stability of Lipid siRNA Nanoparticles: Examining the Effect of pH, Temperature, and Lyophilization — ***Rebecca Ball,*** *Palak Bajaj, Kathryn A. Whitehead*

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(599) Dynamic Simulation and Optimization
Wednesday, Nov 1, 3:15 PM
MCC, 103E

Ali Mesbah, Chair
Ravendra Singh, Co-Chair
Dimitrios I. Gerogiorgis, Co-Chair

Sponsored by:
Computers in Operations and Information Processing

3:15 Paper 599a: Exploiting Structure in Direct Simultaneous Methods for Global Dynamic Optimization — *Yukun Wang, Jai Rajyaguru,* ***Benoit Chachuat***

3:34 Paper 599b: Demand Response Operation of Air Separation Units Utilizing an Efficient MILP Modeling Framework — ***Morgan Kelley,*** *Richard Pattison, Ross Baldick, Michael Baldea*

3:53 Paper 599c: Automatic Sensitivity Analysis and Structure-Exploiting Nonlinear Programming for Dynamic Optimization — ***Joel A. E. Andersson***

4:12 Paper 599d: Dynamic Modelling of an LNG Storage Tank in a Regasification Terminal — ***Surya Effendy,*** *Mohd S. Khan, Shamsuzzaman Farooq, Iftekar A. Karimi*

4:31 Paper 599e: Optimization of Dynamic Flux Balance Analysis Systems — ***Jose A. Gomez,*** *P. I. Barton*

4:50 Paper 599f: Parallel Cyclic Reduction Decomposition for Dynamic Optimization Problems — *Wei Wan,* ***John P. Eason,*** *Bethany Nicholson, Lorenz T. Biegler*

5:09 Paper 599g: Dynamic Optimization of Polymerization Processes with Detailed Molecular Weight Distributions — ***John P. Eason,*** *Yannan Ma, Xi Chen, Lorenz T. Biegler*

5:28 Paper 599h: Improved Bounds on the Solutions of Nonlinear Dynamic Systems Using Centered-Form Differential Inequalities — *Kai Shen,* ***Joseph Scott***

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(600) Efficient Processing of Lignin to Bioproducts and Biofuels II
Wednesday, Nov 1, 3:15 PM
MCC, 103B

Bin Yang, Chair

Sponsored by: Innovations of Green Process Engineering for Sustainable Energy and Environment

3:15 Paper 600a: Effect of Carbonaceous Susceptors on Selective Production of Phenolics and Syngas from Lignin via Microwave Pyrolysis — ***A. Yerrayya,*** *Dadi V. Suriapparao, R. Vinu*

3:37 Paper 600b: Catalytic Conversion of Lignin in Ionic Liquids via Catalysis and Biocatalysis — *Lalitendu Das, Joseph Stevens, Enshi Liu,* ***Jian Shi***

3:59 Paper 600c: Depolymerization of Lignin Using Peracetic Acid Under Mild Conditions — ***Chang Geun Yoo,*** *Yunqiao Pu, Arthur J. Ragauskas*

4:21 Paper 600d: Low-Energy Catalytic Electrolysis for Simultaneous Hydrogen Evolution and Lignin Depolymerization — ***Xu Du,*** *Wei Liu, Zhe Zhang, Arie Mulyadi, Alex Brittain, Yulin Deng*

4:43 Paper 600e: Co-Optimization of Lignin and Carbohydrate Processability by Combinatorial Pretreatment — ***Zhi-Hua Liu,*** *Michelle L. Olson, Yunqiao Pu, Katy Kao, Arthur J. Ragauskas, Mingjie Jin, Joshua Yuan*

5:05 Paper 600f: Cleavage of β-O-4 Ether Bonds in Acidic Lithium Bromide Trihydrate for Lignin Depolymerization — ***Ning Li,*** *Xiaohui Yang, Xuliang Lin, Xuejun Pan*

5:27 Paper 600g: Oxidative Functionalization of Lignins for the Synthesis of Polyamides and Polyesters — ***Zhenglun "Glen" Li***

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(601) Energy System Design II
Wednesday, Nov 1, 3:15 PM
MCC, 103C

Parag Jain, Chair
Alexander W. Dowling, Co-Chair
Nagore Sabio, Co-Chair

Sponsored by:
Systems and Process Design

3:15 Paper 601a: A Mathematical Programming Approach for Integrating Distributed Urban Energy Systems and IoT — ***Nagore Sabio,*** *Evgenia Mechleri, Harvey Arellano-Garcia*

3:36 Paper 601b: Life-Cycle Optimization of Shale Gas Supply Chains with Comprehensive Environmental Impacts and Modeling of Modular Plants — ***Jiyao Gao,*** *Fengqi You*

3:57 Paper 601c: Unit Commitment Operation of Energy Storage Systems: Comparison of Multi-Stage Stochastic Programming and EMPC — ***Oluwasanmi Adeodu,*** *Donald J. Chmielewski*

4:18 Paper 601d: Cooling Limitations in Power Plants: Optimal Multiperiod Design of Natural Draft Cooling Towers — ***Mariano Martin,*** *Mónica Martín*

4:39 Paper 601e: Dynamic Process Modeling for a 10 MWe Supercritical CO_2 Recompression Brayton Pilot Plant Design — ***Stephen E. Zitney,*** *Eric A. Liese, Priyadarshi Mahapatra, Jacob Albright, Debangsu Bhattacharyya*

5:00 Paper 601f: Systematic Integration of Carbon Capture, Utilization and Storage Technologies to Meet CO_2 Emission Reduction Targets — ***Emre Gençer,*** *Francis O'Sullivan*

5:21 Paper 601g: Representative Energy Costs for Optimization of Industrial Process Design and Operations: Systematic Comparison of Clustering Methodologies — ***Holger Teichgräber,*** *Adam Brandt*

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(602) Fate, Transport, and Remediation of Contaminants in the Environment
Wednesday, Nov 1, 3:15 PM
MCC, 200F

Megan A. Creighton, Chair
Jennifer Guelfo, Co-Chair

Sponsored by:
Transport and Energy Processes

3:15 Paper 602a: Fluorescence-Based Detection of Polychlorinated Biphenyls in Water — ***Irfan Ahmad,*** *J. Zach Hilt, Thomas Dziubla*

3:31 Paper 602b: Calorimetric Method for Monomer SAPT Transportation Regulation — ***Min Sheng,*** *Steve Horsch, Florin Dan, Robert Bellair, Marabeth Holsinger*

3:47 Paper 602c: Soil Amendments Used During Remediation of Contaminated Sites Enhance Plant Growth but Increase Mobility of Chrysotile Fibers in One Case — *Cedric Gonneau, Sanjay Mohanty, Jane Willenbring,* ***Brenda Casper***

4:03 Paper 602d: Phosphorus Loading and Speciation Dynamics in Runoff Sediments Moving Through a Eutrophic Watershed: Prospecting a Potentially Recoverable Nutrient Resource — ***Katie Gaviglio,*** *Andro Mondala*

4:19 Paper 602e: The Influence of Suspended Sediment on Electrochemical Remediation of Karst Groundwater — ***Kimberly Hetrick,*** *Ljiljana Rajic, Dorothy Vesper, Ingrid Padilla, Akram Alshawabkeh*

4:35 Paper 602f: Development of an Analytical Modeling Framework for Matrix Diffusion in Multi-Layered Systems — ***Jay Thompson,*** *Eric Tollefsrud*

4:51 Paper 602g: Synthesis and Characterization of Fluorescent Polymers for the Detection of Polychlorinated Biphenyls — ***Dustin Savage,*** *J. Zach Hilt, Thomas D. Dziubla*

5:07 Paper 402l: The Benefits of Research Translation to Environmental Research: A Case Study Featuring Fate and Transport of per- and Polyfluoroalkyl Substances in New England — ***Jennifer Guelfo,*** *Eric M. Suuberg*

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(603) Fundamentals of Electrode Processes III
Wednesday, Nov 1, 3:15 PM
MCC, M100C

Hong Yang, Chair
Gang Wu, Co-Chair
William E. Mustain, Co-Chair

Sponsored by:
Electrochemical Fundamentals

3:15 Paper 603a: Molybdenum Dioxide–Functionalized CoP Porous Nanocatalyst for Highly Efficient Hydrogen Evolution — *Jun Wang,* ***Liang-Xin Ding,*** *Haihui Wang*

3:35 Paper 603b: Bijel-Derived Materials for Electrochemical Energy Storage and Conversion — *Kyle McDevitt, Daniel R. Mumm,* ***Ali Mohraz***

3:55 Paper 603c: Electrochemical Lithiation-Delithiation of Sulfur in Sub-Nano Confinement — *Chengyin Fu,* ***Juchen Guo***

4:15 Break

4:25 Paper 603d: Durable High-Capacity Li-O_2 Cathode Composed of Iron-Nitrogen-Doped Mesoporous Core-Shell Carbon Loaded with RuO_2 Nanoparticles — *Ming Zhou,* ***Kwong-Yu Chan,*** *Chi-Ying Vanessa Li*

4:45 Paper 603e: Magnetic Field-Induced Fabrication of Fe_3O_4@ Graphene Nanocomposites for Enhanced Electrode Performance in Lithium-Ion Batteries — ***Huan Wang,*** *Jingyi Xie, Marissa Follette, Tyson C. Back, Placidus B. Amama*

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(604) Halide Perovskite Synthesis and Applications
Wednesday, Nov 1, 3:15 PM
MCC, 210A/B

Aaron T. Fafarman, Chair
Matthew G. Panthani, Co-Chair

Sponsored by:
Electronics and Photonics

3:15 Paper 604a: Highly Stable Perovskite Solar Cells Fabricated Using Aerosol-Based Technique — ***Shalinee Kavadiya,*** *Pratim Biswas*

3:35 Paper 604b: Engineering Perovskite Solar Cell Interfaces to Realize > 1000 Hr, Unencapsulated Ambient Stability — ***Jeffrey A. Christians,*** *Philip Schulz, Jonathan Tinkham, Tracy H. Schloemer, Bertrand Tremolet de Villers, Steve Harvey, Alan Sellinger, Joseph J. Berry, Joseph M. Luther*

3:55 Paper 604c: A Thermodynamic Basis for Engineering Enhanced Stability of the Perovskite Phase of Cesium Lead Iodide — *Subham Dastidar,* ***Aaron T. Fafarman***

4:15 Paper 604d: Synthesis of Nanostructured Inorganic Perovskites for Solar Cell Applications — ***Atefe Hadi,*** *Rainie D. Nelson, Iver J. Cleveland, Jeremy M. Jacoby, Matthew G. Panthani*

4:35 Break

4:45 Paper 604e: Discovery of Near-Infrared-Active Colloidal Multinary Lead Halide Perovskite Nanocrystals Using a Microfluidic Platform — ***Ioannis Lignos,*** *Viktoriia Morad, Richard Maceiczyk, Loredana Protesescu, Maksym V. Kovalenko, Andrew J. deMello*

5:05 Paper 604f: Improved Charge Collection in Highly Efficient $CsPbBrI_2$ Solar Cells with Light-Induced Dealloying — *Joshua Choi*

5:25 Paper 604g: Synthesis and Characterization of Bi-Based Perovskite Semiconductors for Photovoltaic Application — ***Umar H. Hamdeh,*** *Rainie D. Nelson, Bradley J. Ryan, Ujjal Bhattacharjee, Jacob W. Petrich, Matthew G. Panthani*

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(605) HIDiC Applications and Reactive Distillation
Wednesday, Nov 1, 3:15 PM
MCC, M100G

Daniel R. Summers, Chair
Andrew W. Sloley, Co-Chair
Clint P. Aichele, Co-Chair

Sponsored by:
Distillation and Absorption

3:15 Paper 605a: Heat Transfer Investigation and Dynamic Simulation of Internally Heat-Integrated Distillation Column — ***Chunli Li,*** *Jing Fang, Junjie Qi, Weiyi Su, Hao Li*

3:40 Paper 605b: Performance Improvement of an Intensified Heat Integration Scheme: Reactive Pressure Swing Distillation — ***Bandaru Kiran***

4:05 Paper 605c: Experimental Study in a Reactive Dividing-Wall Column Based on Ethyl Acetate Synthesis — ***Jiangwei Xie,*** *Chunli Li, Fei Peng, Jing Fang, Honghai Wang*

4:30 Paper 605d: Operation of Reactive Distillation Columns Disproportionating Trichlorosilane to Silane: Dynamic Impact of the Number of Reactive Sections — *Kejin Huang, Haisheng Chen, Yang Yuan,* ***Xinxiang Zang,*** *Shaofeng Wang, Liang Zhang*

4:55 Paper 605e: A Novel Potential Application of SiC Ceramic Foam Material to Distillation: Foam Monolithic Tray — ***Xin Gao,*** *Hong Li, Xingang Li*

5:20 Paper 605f: Case Study: Comparison of Energy Consumptions in CDU Complex for Different Pre-Heating Configurations

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(606) In Honor of Jim Rawlings's 60th Birthday
Wednesday, Nov 1, 3:15 PM
MCC, 103D

Victor M. Zavala, Chair
Christopher V. Rao, Co-Chair

Sponsored by:
Systems and Process Control

3:15 Paper 606a: Finding the Optimal Path — ***Thomas F. Edgar***

3:35 Paper 606b: Model Predictive Control and Estimation: Towards Decision Making in the Cloud — ***Rolf Findeisen,*** *Sergio Lucia, Lisa Cairus*

3:55 Paper 606c: OffSet-Free Tracking: There and Back Again — ***Gabriele Pannochia***

4:15 Paper 606d: Linking Stability and Robustness of Nonlinear MPC and Economic MPC to Properties of Optimization Subproblems: Building on the Rawlings Results — ***Lorenz Biegler***

4:35 Paper 606e: Adventures in Model Predictive Control: Tales from a 30-Year Collaboration with Professor Jim Rawlings — ***Thomas A. Badgwell***

4:55 Paper 606f: Model Predictive Control and Moving Horizon Estimation — ***Christopher V. Rao***

5:15 Paper 606g: Discussions on Scheduling, (Re)Optimization, Feedback, and Closed-Loop Performance — ***Christos Maravelias***

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(607) KIChE-US Chapter Open Forum (Invited Talks)
Wednesday, Nov 1, 3:15 PM
MCC, 102F

Jaehun Chun, Chair
Su Ha, Co-Chair
Hyunmin Yi, Co-Chair
Tae-Sik Oh, Co-Chair

Sponsored by: International Committee

3:15 Introductory Remarks

3:25 Paper 607a: Computational Materials Design for Developing High-Performance Solid Oxide Fuel Cell Electrodes — ***Jeong Woo Han***

3:45 Paper 607b: Systems Biotechnology for Understanding and Designing Microbial, Plant and Mammalian Cell Factories — ***Dong-Yup Lee***

4:05 Paper 607c: Integration of Iterative Learning Control and Model Predictive Control for Point-to-Point Tracking Problem — *Se-Kyu Oh,* ***Jong Min Lee***

4:25 Paper 607d: First-Principles Modeling of Redox Potential of Organic Materials for Lithium-Ion Batteries — ***Seung Soon Jang***

4:45 Award Ceremony, Presentation, and Lectures

4:46 Paper 607e: Doh Wonsuk Award

5:06 Paper 607f: Correlating Molecular Details to Emergent Phenomena for Colloidal Dispersions — ***Jaehun Chun***

5:26 Paper 607g: Interfacial Dynamics of Ionic Liquids Under Nanoconfinement — ***Younjin Min***

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(608) Membrane Reactors
Wednesday, Nov 1, 3:15 PM
MCC, 101D

Theodore Tsotsis, Co-Chair
Shamsuddin Ilias, Co-Chair
Dolly Chitta, Co-Chair

Sponsored by:
Membrane-Based Separations

3:15 Paper 608a: Experimental and Simulation Studies of High-Temperature Ethane Dehydrogenation in Microporous Zeolite Membrane Reactor — *Shailesh Dangwal, Ruochen Liu,* ***Seok-Jhin Kim***

3:35 Paper 608b: Experimental and Numerical Study of an Intensified Water-Gas Shift (WGS) Reaction Process Using a Membrane Reactor (MR)/Adsorptive Reactor (AR) Sequence — ***Huanhao Chen****, Mingyuan Cao, Secgin Karagoz, Vasilios Manousiouthakis, Theodore Tsotsis*

3:55 Paper 608c: Synthesis & Performance Study of Pd-Au/PSS Membrane Reactor to Produce Highly Pure Hydrogen via Natural Gas Steam Reforming — ***Simona Liguori****, Bryce Anzelmo, Yi-Hua Ma, Ivan Mardilovich, Jennifer Wilcox*

4:15 Paper 608d: Non-Isothermal CFD Study of Ethanol Steam Reforming in a Catalytic Membrane Reactor — ***Rui Ma****, Bernardo Castro Dominguez, Anthony G. Dixon, Yi Hua Ma*

4:35 Paper 608e: Enhanced Performance of $La_{0.6}Sr_{0.4}Co_{0.2}Fe_{0.8}O_3$ (LSCF) Membranes by Atomic Layer Deposition of a Protecting Alumina Nanofilm — *Peter J. King, Guangru Zhang, Anthony O'Neill,* ***Ian S. Metcalfe***

4:55 Paper 608f: Improving Dehydrogenation Conversion and Selectivity by Utilizing Thermally Stable Membranes — ***Yixiao Li****, Mary E. Rezac, Leslie Schulte*

5:15 Paper 608g: Integration of Synthesized Catalysts and Membrane in Packed- and Fluidized-Bed Membrane Reformer for Production of Hydrogen Through Steam Reforming — ***Richa Sharma****, Amit Kumar, Rajesh Kumar Upadhyay*

5:35 Paper 608h: Novel Eductor-Based MBR with Enhanced Mass Transfer and Fouling Resistance for the Treatment of Domestic Wastewater — ***Shibam Mitra****, Naphtali Daltrophe, Jack Gilron*

(609) Microbial Communities and Microbiomes for Agriculture and Bioenergy

Wednesday, Nov 1, 3:15 PM
MCC, 205A/B

Chase L. Beisel, Chair

Sponsored by: Microbiomes and Microbial Communities

3:15 Paper 609a: Engineering Cross-Feeding Co-Cultures as a Platform for High-Throughput Screening of Microbial Strain Libraries for Enhanced Biomolecule Production — ***Tatyana Saleski****, Azzaya Khasbaatar, Xiaoxia (Nina) Lin*

3:40 Paper 609b: Engineering Microbial Consortia for Bioelectrocatalysis Processes — ***Hao Song***

4:05 Paper 609c: Screening Rhizobacteria Interactions Using a High-Throughput Microwell Array Platform — ***Ryan Hansen****, Andre van der Vlies, Niloy Barua, Logan McGinely, Niloufar Fattahi, Tom Platt*

4:30 Paper 609d: Engineering Modular Microbial Communities for Cellulose Utilization and Bioproduct Synthesis — ***Karolina Z. Kalbarczyk****, Cynthia H. Collins, Mattheos A. G. Koffas*

4:55 Paper 609e: Symbiotic Microbial Communities for Cleaning Agricultural Waters and Bioenergy Production — ***Aravindan Rajendran****, Bruno Hespanhol, Tanner Barnharst, Cristiano Reis, Bo Hu*

(610) Mixed-Matrix Membranes for Gas Separation — GS III

Wednesday, Nov 1, 3:15 PM
MCC, M100I

W. S. Winston Ho, Co-Chair
Haiqing Lin, Co-Chair
Yan Wang, Co-Chair

Sponsored by: Membrane-Based Separations

3:15 Paper 610a: Facile Fabrication of Ultrathin Molecular Sieving ZIF-8 Hollow Fiber Membranes on Polydopamine-Polyethyleneimine-Coated Microporous PVDF Supports — *Putu Sutrisna, Jingwei Hou, Hao-Cheng Yang, Hongyu Li,* ***Vicki Chen***

3:37 Paper 610b: Effect of Graphene Oxide on Gas Transport and Sorption in Poly(dimethylsiloxane)-Based Membranes — ***Jaesung Park****, Heonjoo Ha, Hee Wook Yoon, Melanie M. Merrick, Ho Bum Park, Christopher J. Ellison, Benny D. Freeman*

3:59 Paper 610c: Tailoring Interfacial Properties in Mixed-Matrix Membranes via Supramolecular Interactions — ***Qinnan Zhang****, Ruilan Guo*

4:21 Paper 610d: Chemical Vapor Deposition on Chabazite (CHA) Zeolite Membranes for Improving CO_2/N_2 Separation Performance — ***Yanghwan Jeong****, Jungkyu Choi*

4:43 Paper 610e: Molecular Dynamics Simulation of Mixed-Matrix Membrane Formed by Porous Organic Cage and Polymer with Intrinsic Microporosity — ***Xian Kong****, Jianwen Jiang*

5:05 Paper 610f: High-Performance Composite Membrane for Olefin/Paraffin Separation — ***Zhong Tang****, Lin-Feng Li*

5:27 Paper 610g: Comparative Study of Two Nano-Composite Membranes for Efficient CO_2 Removal — ***Ahmad Arabi Shamsabadi****, Farzad Seidi, Ehsan Salehi, Mohammad Nozari, Ahmad Rahimpour, Masoud Soroush*

(611) Mixing Award Session

Wednesday, Nov 1, 3:15 PM
MCC, 102D

David S. Dickey, Chair
Otute Akiti, Co-Chair

Sponsored by: North American Mixing Forum

3:15 Paper 611a: Mixing Award Presentation — ***David S. Dickey****, Otute Akiti*

(612) Modeling and Control of Crystallization

Wednesday, Nov 1, 3:15 PM
MCC, M100J

Meenesh R. Singh, Chair
Lotfi Derdour, Co-Chair
Michael Lovette, Co-Chair

Sponsored by: Crystallization and Evaporation

3:15 Introductory Remarks

3:20 Paper 612a: Calculation of Free-Energy Barriers for Attachment of Molecules During Crystal Growth and Nucleation — ***Anish V. Dighe****, Meenesh R. Singh*

3:40 Paper 612b: Population Balance Modeling and Optimization of an Integrated Batch Crystallizer–Wet Mill System for Crystal Size Distribution Control — ***Botond Szilagyi****, Zoltan K. Nagy*

4:00 Paper 612c: A Cellular Automata Approach for Simulation of Crystal Growth — ***Jiaying Ke****, B. Erik Ydstie, Aditya S. Khair*

4:20 Paper 612d: Optimal Crystal Size Control Using a Continuous Plug-Flow Crystallization Configuration with Recycle — ***Xiaodong Xu****, Yuan Yuan, Stevan Dubljevic*

4:40 Paper 612e: Multiphysics Modeling and Simulation of Microfluidic Platforms for Screening of Pharmaceutical Polymorphs — ***Paria Coliaie****, Meenesh Singh*

5:00 Paper 612f: Motion-Based Multiple-Object Tracking of Ultrasonic-Induced Nucleation: A Case Study of L-Glutamic Acid — *Zhenguo Gao, Dan Zhu, Yuanyi Wu,* ***Sohrab Rohani****, Junbo Gong, Jingkang Wang*

5:20 Concluding Remarks

(613) Modeling of Lipid Membranes and Membrane Proteins

Wednesday, Nov 1, 3:15 PM
MCC, L100I

Shikha Nangia, Chair
Shivangi Saurabh, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

3:15 Paper 613a: Elucidating Mechanisms of Substrate Transport in Membrane Transporters — ***Diwakar Shukla****, Balaji Selvam*

3:30 Paper 613b: Grafting Charged Species to Membrane-Embedded Scaffolds Dramatically Increases the Rate of Bilayer Translocation — ***Reid Van Lehn***

3:45 Paper 613c: Molecular Simulations of Nanoparticles Permeating Lipid Membranes for Drug Delivery Applications — ***Priyanka Oroskar****, Cynthia J. Jameson, Sohail Murad*

4:00 Paper 613d: Transport Characteristics and Stability of Artificial Water Channels in Lipid and Biomimetic Membranes — ***Harish Vashisth***

4:15 Paper 613e: Solute Transport Through Outer Membrane Porins of Gram-Negative Bacteria — ***Huilin Ma****, Aliza Khan, Shikha Nangia*

4:30 Paper 613f: Could Class-IIb Bacteriocins Induce Pore Formation? Investigation Through Microsecond Long Atomistic Molecular Dynamic Simulation — ***Panagiota Kyriakou****, Yiannis N. Kaznessis*

4:45 Paper 613g: Host-Pathogen Interactions at the Tight Junctions: Molecular Insights from Membrane-Guided Self-Assembly — ***Flaviyan Jerome Irudayanathan****, Xiaoyi Wang, Nan Wang, Shikha Nangia*

5:00 Paper 613h: Structure of Multi-Component, Gel-Phase Lipid Bilayers — ***Alexander Yang****, Timothy C. Moore, Christopher R. Iacovella, Michael Thompson, Pallav Bulsara, David J. Moore, Clare McCabe*

5:15 Paper 613i: Multiplicity of States and Internal Structure of Supported Lipid Bilayers — *Aleksey Vishnyakov, Ting Li,* ***Alexander V. Neimark***

5:30 Paper 613j: Line Tension and Lipid Sorting Modulate Dynamics of Hemifusion Diaphragm Dissipation — ***Jasmine Gardner****, Cameron F. Abrams*

(614) Molecular Simulation of Adsorption I — In Honor of Keith Gubbins's 80th Birthday III (Invited Talks)

Wednesday, Nov 1, 3:15 PM
MCC, M100E

Alexander V. Neimark, Chair
Gennady Gor, Co-Chair

Sponsored by: Adsorption and Ion Exchange

3:15 Paper 614a: Understanding the Removal of Pharmaceuticals from Water Effluents by Adsorption in Activated Carbons: A Molecular Simulation Approach — ***Lourdes F. Vega****, Daniel Bahamon*

3:35 Paper 614b: Insights into the Adsorption and Phase Behaviour of Fluids in Nanoporous Materials with Hierarchical Pore Structure: Towards an Advanced Textural Characterization — ***Matthias Thommes***

3:55 Paper 614c: Molecular Studies of Supercapacitors: Ionic Liquids Adsorbed into Porous Carbon Electrodes — ***Peter T. Cummings***

4:15 Paper 614d: Structure of Ice in Confinement; Water in Mesopores — ***Malgorzata Sliwinska-Bartkowiak***

4:35 Paper 614e: Towards Understanding the Role of Microstructure in Energetic Material Response: Coarse-Grain Modeling and Simulation — ***John K. Brennan***

4:55 Break

5:15 Paper 614g: Adsorption and Transport in Multiscale Porous Media — ***Benoit Coasne***

(615) Nanobiotechnology for Sensors and Imaging II

Wednesday, Nov 1, 3:15 PM
MCC, 212A/B

Venkat R. Bhethanabotla, Chair
Subramanian Sankaranarayanan, Co-Chair
Daniel Roxbury, Co-Chair

Sponsored by: Bionanotechnology

3:15 Paper 615a: To COIN a Term: Functional Composite Organic-Inorganic Nanoparticles (COINs) for Biomedical Applications — ***Brian K. Wilson****, Robert K. Prud'homme*

3:33 Paper 615b: Combined MPI-MFH: A Promising Theranostic Platform — ***Rohan Dhavalikar****, Daniel Hensley, Zhi Wei Tay, Bo Zheng, Patrick W. Goodwill, Steven M. Conolly, Carlos Rinaldi*

3:51 Paper 615c: Folate-Targeted Semiconducting Polymeric Patchy Particles: Potential Tool for Photoacoustic Imaging and Drug Delivery — *Binal Brahmbhatt, Kaitlyn Scott, Veda Prasad, Dora Obodo, Amr Majul, Sundaresan Gobalakrishnan, Jamal Zweit,* ***Carolina Salvador-Morales***

4:09 Paper 615d: Identification of Amino Acids for Templating Gold Nanoparticles Under Low Doses of Ionizing Radiation: From Discovery to Design — ***Karthik Pushpavanam****, Sahil Inamdar, Tomasz Bista, Stephen Sapareto, Kaushal Rege*

4:27 Paper 615e: Modeling the Response of Magnetic Nanoparticles Relaxing by the Neel Mechanism for Magnetic Particle Imaging — ***Rohan Dhavalikar****, Carlos Rinaldi*

4:45 Paper 615f: A Stomatal Electro-Mechanical Pore Size Sensor (SEMPSS) for Persistent Monitoring of Plant Physiology — ***Volodymyr Koman****, Tedrick Salim Lew, Min Hao Wong, Seon-Yeong Kwak, Michael Strano*

5:03 Paper 615g: Biocompatibility of ZnO Thin Films for Sensor Applications — ***Nastassja Lewinski****, Vitaliy Avrutin, Tanin Izadi, Barkat Ullah, Umit Ozgur, Hadis Morkoc, Erdem Topsakal*

5:21 Paper 615h: Highly Stable and Near-UV Activated $YVO_4:Eu^{3+},Bi^{3+}$ Nanophosphors for Bioimaging and In-Vitro Dosimetry — ***Anastasia Spyrogianni****, Peter G. Tiefenboeck, Frank Krumeich, Jean-Christophe Leroux, Sotiris E. Pratsinis, Georgios A. Sotiriou*

(616) Nanofabrication and Nanoscale Processing

Wednesday, Nov 1, 3:15 PM
MCC, 213A/B

Hebab Quazi, Chair
Evan K. Wujcik, Co-Chair
Kevin J. Cash, Co-Chair

Sponsored by: Nanoscale Science and Engineering Forum

3:15 Paper 616a: Tunable Hollow Gold Nanoshell Structures of Varying Morphology Formed Using Soft Core-Shell Templates — ***Geoffrey D. Bothun****, Akram Abbasi, Arijit Bose, Keunhan Park*

3:33 Paper 616b: Increasing the Hydrophobicity of Biologic Active Pharmaceutical Ingredients by Generating Insoluble Salt Forms to Enable Continuous Nanoprecipitation and Encapsulation — ***Kurt D. Ristroph****, Hoang Lu, Paradorn Rummaneethorn, Robert Prud'homme*

3:51 Paper 616c: Crosslinked Hairy Nanoparticle Membrane for Enabling High Reversibility in Lithium-Metal Batteries — ***Snehashis Choudhury****, Lynden A. Archer*

4:09 Paper 616d: High-Throughput Polymeric Nanoparticles Synthesis via Flash Nanoprecipitation — ***Kil Ho Lee****, Matthew S. Souva, Barbara E. Wyslouzil, Jessica O. Winter*

4:27 Paper 616e: Green Synthesis of Ag & Pd Nanostructures — ***Shohreh Hemmati****, Erin Retzlaff-Roberts, Corren Scott, Michael T. Harris*

4:45 Paper 616f: Nanofabrication of Devices for Electromagnetic Energy Capture and Conversion to Electricity — ***Patrick J. Pinhero****, Zachary Thacker*

5:03 Paper 616g: Free-Standing Sulfur/Carbon Nanofibers Film as a Cathode for Lithium-Sulfur Battery — *Xiong Song,* ***Suqing Wang****, Haihui Wang*

5:21 Paper 616h: Influence of Surface Asperities and Surface Energetics on Wetting Characteristics of Spherical Glass Beads — ***Deepa Dixit****, Chinmay Ghoroi*

(617) Nanostructured Thin Films

Wednesday, Nov 1, 3:15 PM
MCC, 209A/B

Ke Zhang, Chair
Seok-Jhin Kim, Co-Chair

Sponsored by: Inorganic Materials

3:15 Paper 617a: In-Situ Synthesis of Intergrown UiO-66 Membranes with Controlled Orientation — ***Bohan Shan****, Bin Mu*

3:33 Paper 617b: Closed-Packed, Oriented MOF Thin Films Through Solution Shearing — ***Arian Ghorbanpour****, Luke Huelsenbeck, Gaurav Giri*

3:51 Paper 617c: Mechanistic Insights into Low-Temperature Ceramic Thin-Film Growth and Crystallization Using Microwave Radiation — ***B. Reeja Jayan****, Nathan Nakamura*

4:09 Paper 617d: Gold Nanoparticle Monolayers for Surface-Enhanced Raman Spectroscopy of Lithium Batteries — ***Daniel T. Hallinan Jr.****, Guang Yang, Jagjit Nanda, Boya Wang, Gang Chen*

4:27 Paper 617e: Understanding the Chemistry of Thiol-Amine Solutions: Versatile Solvents for Solution-Processed Thin-Film Photovoltaics — ***Caleb Miskin****, Priya Murria, Laurance Cain, Robert W. Boyne, Evan C. Wegener, Jeffrey T. Miller, Hilkka Kenttamaa, Rakesh Agrawal*

4:45 Paper 617f: In-Situ Grazing Incidence Small-Angle X-Ray Scattering (GISAXS) Study of the Formation of Multilayered Ordered Mesoporous Titania Films — ***M. Arif Khan****, Syed Z. Islam, Suraj Nagpure, Barbara L. Knutson, Stephen E. Rankin*

5:03 Paper 617g: 2-D Wulff Construction of FeOx Islands Grown on Pt(111) for Use in Catalysis — ***Joseph Kubal****, Jeffrey Greeley*

(618) NH_3 Fuel End Use and Synthesis

Wednesday, Nov 1, 3:15 PM
MCC, 101F/G

Sponsored by: NH_3 Energy⁺ — Enabling Optimized, Sustainable Energy and Agriculture

3:15 Paper 618a: Methods for Low-NOx Combustion in Ammonia/Natural Gas Dual-Fuel Gas Turbine Combustor — ***Shogo Onishi****, Shintaro Ito, Masahiro Uchida, Soichiro Kato, Tsukasa Saito, Toshiro Fujimori, Hideaki Kobayashi*

3:33 Paper 618b: $NH_3/N_2/O_2$ Non-Premixed Flame in a 10 kW Experimental Furnace: Characteristics of Radiative Heat Transfer — ***Ryuichi Murai****, Ryohei Omori, Ryuki Kano, Yuji Tada, Hidetaka Higashino, Noriaki Nakatsuka, Jun Hayashi, Fumiteru Akamatsu, Kimio Iino, Yasuyuki Yamamoto, Yoshiyuki Hagiwara*

3:51 Paper 618c: Delivering Clean Hydrogen Fuel from Ammonia Using Metal Membranes — ***Michael D. Dolan***

4:09 Paper 618d: Novel Catalysts for Ammonia Cracking and Synthesis — ***William David****, Josh Makepeace, Thomas Wood*

4:27 Paper 618e: Future of Ammonia Production: Improvement of Haber-Bosch Process for Electrochemical Synthesis? — ***Grigorii Soloveichik***

4:45 Paper 618f: Fast-Ramping Reactor for CO_2-Free NH_3 Synthesis — ***Joseph Beach****, Jonathan Kintner, Adam Welch, Jason Ganley, Ryan O'Hayre*

5:03 Paper 618g: Lower-Pressure Ammonia Synthesis — ***Mahdi Malmali****, Mike Reese, Alon V. McCormick, Edward L. Cussler, Joshua Prince*

5:21 Paper 618h: Nitrogenase-Inspired Peptide-Functionalized Catalyst for Efficient, Emission-Free Ammonia Production — ***Stephen Szymanski***, *Wayne Gellett*

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(619) NSF Workshop II: Proposal Writing and Discussions with Program Managers
Wednesday, Nov 1, 3:15 PM
MCC, 101H

William L. Olbricht, Chair
Ram B. Gupta, Co-Chair

Sponsored by: Graduate Education

3:15 Paper 619a: Proposal Writing Tutorial — ***William L. Olbricht***

4:15 Paper 619b: Interactive Breakout Panels — ***Carole Read***, *Steven Peretti, Bruce Hamilton, Robert W. McCabe, T. J. Mountziaris*

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(620) Particle Technology Awards Lectures
Wednesday, Nov 1, 3:15 PM
MCC, 200H

Rajesh N. Dave, Chair
Bruce D. Hook, Co-Chair

Sponsored by: Particle Technology Forum

3:15 Introductory Remarks

3:20 Paper 620a: Shell Thomas Baron Award Lecture: Exploring Complex Colloidal Dispersions by Simulation — ***Jeffrey F. Morris***

4:10 Paper 620b: Elsevier PTF Lifetime Achievement Award: An Industrial/ Academic Career Full of Learning, Challenge, Opportunity, and Fun — ***Alan W. Weimer***

5:00 Paper 620c: PSRI Lectureship Award in Fluidization: Sand, Waves, Trees and People: A NICE Journey in Fluidization — ***Marc-Olivier Coppens***

5:50 Concluding Remarks

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(621) Polymer Crystallization
Wednesday, Nov 1, 3:15 PM
MCC, 211C

Ying Diao, Chair
Jian Qin, Co-Chair

Sponsored by: Polymers

3:15 Paper 621a: Molecular Simulation of Crystallization of Chain Molecules from the Melt — ***Gregory C. Rutledge***

3:45 Paper 621b: Anomalous Crystallization Behavior of Ring Polymers — ***Kiran S. Iyer***, *Murugappan Muthukumar*

4:00 Paper 621c: Thin-Film Crystallization of Cyclic Polymers and Their Linear Analogues — ***Julie Albert***, *Giovanni Kelly, Scott Grayson, Farihah Haque*

4:15 Paper 621d: Synthesis, Characterization, and Structural Evolution of Designer Block Polyelectrolyte Complexes — ***Jeffrey Ting***, *Hao Wu, Abraham Herzog-Arbeitman, Samanvaya Srivastava, Matthew V. Tirrell*

4:30 Paper 621e: Polyelectrolyte Association and Solvation — ***Alexandros Chremos***, *Jack Douglas*

4:45 Paper 621f: Solid- and Liquid-Core Polyelectrolyte Complex Micelles — ***Lorraine Leon***

5:00 Paper 621g: Thermodynamics and Transport Properties of Polyether Blend Electrolytes — ***Alysha Helenic***, *Malgorzata Chwatko, Rodrigo Rodriguez, Kathryn E. Loeffler, C. Buddie Mullins, Nathaniel A. Lynd*

5:15 Paper 621h: Scalable Nanocomposites Synthesis via Electrospray-Mediated Electroemulsification and Flash Nanoprecipitation — ***Kil Ho Lee***, *Barbara E. Wyslouzil, Jessica O. Winter*

5:30 Paper 621i: Unique Crystallization Behavior of Isotactic Polypropylene in the Presence of L-Isoleucine and Its Inhibition and Promotion Mechanism of Nucleation — ***Shicheng Zhao***, *Xiaoshan Peng*

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(622) Polymers for Energy Storage and Conversion
Wednesday, Nov 1, 3:15 PM
MCC, 211D

Matthew D. Green, Chair
Joseph F. Stanzione III, Co-Chair

Sponsored by: Polymers

3:15 Paper 622a: Engineering Vapor-Deposited Polymers for Energy Conversion and Storage — ***Kenneth Lau***

3:45 Paper 622b: Charge Transfer Mechanisms in Organic Radical Polymer Batteries — *Shaoyang Wang, Fei Li,* ***Jodie L. Lutkenhaus***

4:00 Paper 622c: Free Volume–Enhanced Anion-Exchange Membranes from Triptycene Poly(Arylene Ether Sulfone) Copolymers — ***Yoonseob Kim***, *Timothy Swager*

4:15 Paper 622d: Surfactant-Polymer System Optimization in Heterogeneous Model with Mobility Control — ***Nai Cao***, *Pingchuan Dong, Brian McPherson, Xiaoxiao Liu*

4:30 Paper 622e: Breaking the Compensation Effect Within the Vogel-Tammann-Fulcher Equation for Polymer-Based Electrolytes — ***Kyle M. Diederichsen***, *Hilda G. Buss, Bryan D. McCloskey*

4:45 Paper 622f: Carbon Derived from Polymerized Ionic Liquids — ***Rui Sun***, *Kelly M. Meek, Yossef A. Elabd*

5:00 Paper 622g: Tailoring Surface Functionalization of Silica Nanoparticles in Nafion Nanocomposites for Improved Ion Selectively in Vanadium Redox Flow Batteries — ***Allison Jansto***, *Eric M. Davis*

5:15 Paper 622h: Thermally Cross-Linked Poly(acrylic acid) / Reduced-Graphene Oxide Aerogels as a Replacement for Metal-Foil Current Collectors in Lithium-Ion Batteries — ***Han Xiao***, *Joshua Pender, Mackenzie Meece-Rayle, Pedro de Souza, Kyle Klavetter, Heonjoo Ha, Jie Lin, Adam Heller, Christopher J. Ellison, C. Buddie Mullins*

5:30 Paper 622i: Graphene Oxide/ Polybenzimidazole Nanocomposite Membrane for High-Temperature Fuel Cell Application — ***Shobha Mantripragada***, *Md. Tashfin Zayed Hossain, Khondker Sultana, Shamsuddin Ilias, Jianzhong Lou*

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(623) Process Intensification and Advanced Control of Pharmaceutical Processes
Wednesday, Nov 1, 3:15 PM
MCC, 101C

Dimitrios I. Gerogiorgis, Chair
Zoltan K. Nagy, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

3:15 Paper 623a: Technoeconomic Evaluation of Cyclosporine Crystallisation Intensification Using a Cascade of M.S.M.P.R. Crystallisers — *Samir Diab,* ***Dimitrios I. Gerogiorgis***

3:36 Paper 623b: Application of Advanced Process Control Tools in Continuous Processing — ***Stephan Sacher***, *Jakob Rehrl, Julia Kruisz, Otto Scheibelhofer, Isabella Aigner, Michael Martinetz, Patrick R. Wahl, Johannes G. Khinast*

3:57 Paper 623c: Nonlinear First-Principle Model-Based Control of a Continuous Pharmaceutical Manufacturing Process — ***Nima Yazdanpanah***, *Thomas O'Connor, Naresh Pavurala, Sonal Mazumder, Muhammad Ashraf, Celia N. Cruz, Cassandra Taylor, Xiaoming Xu*

4:18 Paper 623d: A Fault-Tolerant Control Design for Real-Time Release in Continuous Manufacturing of Solid Dose Using Direct Compaction — ***Qinglin Su***, *Mariana Moreno, Jianfeng Liu, Sudarshan Ganesh, Yasasvi Bommiready, Marcial Gonzalez, Gintaras V. Reklaitis, Zoltan K. Nagy, Thomas O'Connor, Geng Tian*

4:39 Paper 623e: Intensified Crystallization of Sulfathiazole and Sulfanilamide by Direct Co-Crystal Assembly — ***Kuan-Lin Yeh***, *Tu Lee*

5:00 Paper 623f: Direct Co-Crystal Assembly from Synthesis to Co-Crystallization — ***Ya-Chi Fan***, *Hung-Lin Lee, Tu Lee*

5:21 Paper 623g: Continuous Preparation of 1:1 Haloperidol-Maleic Acid Salt by a Novel Solvent-Free Method Using a Twin-Screw Melt Extruder — ***Tu Lee***, *Hung-Lin Lee, Jaydip M. Vasoya, Marilia de Lima Cirqueira, Kuan-Lin Yeh, Abu T. M. Serajuddin*

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(624) Process Intensification by Enhanced Heat and Mass Transfer
Wednesday, Nov 1, 3:15 PM
MCC, 101E

Kishori Deshpande, Chair
Daniela Ferrari, Co-Chair

Sponsored by: Process Intensification & Microprocess Engineering

3:15 Paper 624a: The Micromixing Performance of Micro-Impinging Stream Reactors and Their Applications in Preparing High-Performance Ultrafine Materials — *Kun-Peng Cheng,* ***Li-Xiong Wen***, *Jian-Feng Chen*

3:40 Paper 624b: Intensification of Cryogenic Lithiation-Borylation Through Use of a High-Heat Transfer Loop Reactor — ***Patrick Heider***, *Wayne Blaylock, Duncan L. Browne, Jayachandran Devaraj, Steven V. Ley, James A. Newby*

4:05 Paper 624c: Design of Novel Microalgal Photobioreactor Using Computational Fluid Dynamics — ***Arpit Mishra***, *Geetanjali Yadav, Parthasarthi Ghosh, Ramkrishna Sen*

4:30 Paper 624d: Process-Intensified and Direct Production of Gasoline from Syngas — ***Xinquan Cheng***, *William R. Yantz Jr., Bruce Tatarchuk*

4:55 Paper 624e: Modelling of Time-Dependent Interfacial Properties Due to Chemical Equilibrium Reactions in Demixed Fluid Systems — ***Andreas Danzer***, *Sabine Enders*

5:20 Paper 624f: Impact of Internals on Bubble Column Performance — ***Sai Sankar Ganesan***

(625) Process Monitoring & Fault Detection
Wednesday, Nov 1, 3:15 PM
MCC, 103F

Jeevan Maddala, Chair
Yuncheng Du, Co-Chair

Sponsored by: Data and Information Systems

3:15 Paper 625a: Distributed Fault Diagnosis for Networked Nonlinear Uncertain Systems — ***Hadi Shahnazari***, *Prashant Mhaskar*

3:32 Paper 625b: A Multi-Sensor Error-Detection and Functional Redundancy Algorithm for Dynamic Systems — ***Jianyuan Feng***, *Iman Hajizadeh, Sediqeh Samadi, Mert Sevil, Nicole Frantz, Caterina Lazaro, Zacharie Maloney, Xia Yu, Elizabeth Littlejohn, Laurie Quinn, Ali Cinar*

3:49 Paper 625c: Model-Based Fault Detection for Nonlinear Process Systems Using Multiparametric Programing for Parameter Estimation — ***Ernie Che Mid***, *Vivek Dua*

4:06 Paper 625d: Event Detection and Estimation of Its Influence Based on Fuzzy Qualitative Representation of Measurements and Fuzzy Logic Estimator — ***Sediqeh Samadi***, *Kamuran Turksoy, Iman Hajizadeh, Jianyuan Feng, Mert Sevil, Ali Cinar*

4:23 Paper 625e: Fault Detection and Diagnosis of Continuous Processes via Non-Linear Support Vector Machine-Based Feature Selection — ***Melis Onel***, *Chris A. Kieslich, Yannis A. Guzman, Christodoulos A. Floudas, Efstratios N. Pistikopoulos*

4:40 Paper 625f: Optimal Test Design Framework for Model-Based Active Fault Detection and Isolation — ***Kyle A. Palmer***, *George M. Bollas*

4:57 Paper 625g: Verification of Control Systems with Discrete and Continuous Dynamics — ***Chintan Bhomia***, *Blake C. Rawlings, B. Erik Ydstie*

5:14 Paper 625h: Multi-Rate Sampled-Data Observer Design for Nonlinear Systems with Multiple Measurement Delays — ***Chen Ling***, *Costas Kravaris*

5:31 Paper 625i: Data Reconciliation with Inequality Constraints Induces Bias: A Cause for Concern? — *Kris Villez*

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(626) Protein Engineering III: Rational and Computational Techniques
Wednesday, Nov 1, 3:15 PM
MCC, 207A/B

Philip A. Romero, Chair
Tim Whitehead, Co-Chair

Sponsored by: Bioengineering

3:15 Paper 626a: Flexible-Backbone Protein Docking Using Motif Scoring and Large Conformational Ensembles — ***Shourya S. Roy Burman***, *Nicholas Marze, William Scheffler, David Baker, Jeffrey J. Gray*

3:33 Paper 626b: Systematic Redesigning of *E. coli* water Channel Porin, OmpF, for Desired Pore Size Using Iterative Protein Redesign and Optimization (IPRO) Suite — ***Ratul Chowdhury***, *Tingwei Ren, Karl Decker, Aleksei Aksimentiev, Manish Kumar, Costas Maranas*

3:51 Paper 626c: Rational Methods for Optimizing Antibody Specificity by Controlling the Net Charge of the Complementarity-Determining Regions — *Mark Julian, Lilia Rabia, Kathryn Tiller, Seth Ludwig, Sibel Kalyoncu,* ***Peter Tessier***

4:09 Paper 626d: Insertion of a Calcium-Binding Beta Roll Domain into a Thermostable Alcohol Dehydrogenase Enables Allosteric Control over Cofactor Specificity — ***Walaa Abdallah***, *Kusum Solanki, Scott A. Banta*

4:27 Paper 626e: Engineering a Thioesterase for Improved Medium-Chain Fatty Acid Profile — *Stephen Sarria,* ***Pamela Peralta-Yahya***

4:45 Paper 626f: Leveraging Disulfide Bonds to Stabilize Small Protein Scaffolds During Extensive Diversification — ***Daniel R. Woldring***, *Max A. Kruziki, Benjamin J. Hackel*

5:03 Paper 626g: Next-Generation Therapeutics to Combat Infectious Diseases — ***Jennifer Maynard***

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(627) Protein Structure, Function, and Stability III: Mechanisms
Wednesday, Nov 1, 3:15 PM
MCC, 208A

Nigel Reuel, Chair
Jessica Kelly, Co-Chair

Sponsored by: Bioengineering

3:15 Paper 627a: Understanding the Role of Conformational Change in Product Inhibition of 2-(2' hydroxyphenyl) Benzenesulfinate Desulfinase (DszB) — ***Landon Mills***, *Christina M. Payne, Derek Englert*

3:33 Paper 627b: Structural, Thermodynamics and Kinetics Role of Novel Hot-Spot Mutations of BCR-ABL1 in Resistance Towards "Ibs" Inhibitors — ***Sabrina Pricl***, *Erik Laurini, Maurizio Fermeglia, Domenico Marson, Suzana Aulic, Maurizio Romano, Natasha Skoko, Marco Baralle*

3:51 Paper 627c: Novel Computational Protocol for Small-Molecule–Protein Receptor Docking: Application to 1,4-DHNA and TCDD Binding to AhR Mouse Protein — ***Asuka A. Orr***, *Arul Jayaraman, Stephen Safe, Phanourios Tamamis*

4:09 Paper 627d: Vibrio fischeri Aspartate 1-Decarboxylase Revealed by Model-Enabled Gene Search — ***Shu Pan***, *Kiel Nikolakakis, Edward Ruby, Jennifer Reed*

4:27 Paper 627e: Characterizing the Role of 23S rRNA A- and P-Site Mutations in Translation — ***Tasfia Azim***, *Anne d'Aquino, Michael C. Jewett*

4:45 Paper 627f: Mapping the Aggregation Behaviour of Biopharmaceuticals: A New Approach — ***Sarah Hedberg***, *Jerry Heng, Daryl Williams*

5:03 Paper 627g: Engineering Antimicrobial Peptides to Target Fungal Pathogens — ***Amy J. Karlsson***

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(628) PSA/TSA
Wednesday, Nov 1, 3:15 PM
MCC, M100F

Armin D. Ebner, Chair
Fateme Rezaei, Co-Chair

Sponsored by: Adsorption and Ion Exchange

3:15 Paper 628a: Regeneration of Ammonia-Loaded Metal Halide Absorbents — ***Mahdi Malmali***, *Collin Smith, Alon McCormick, Edward L. Cussler*

3:35 Paper 628b: Development of a TSA Process for Metabolic CO_2 Removal from Spacecraft Cabins Using a Structured 13X Adsorbent — ***James A. Ritter***, *Armin D. Ebner, James C. Knox*

3:55 Paper 628c: PSA-Based CO_2 Capture Above the Dew Point of Synthesis Gas for IGCC Power Plants — ***Ambalavanan Jayaraman***, *Gokhan Alptekin, Michael Bonnema, Chakravarthy Sishtla*

4:15 Paper 628d: On the Development of a PSA Process for Natural Gas Purification — ***James A. Ritter,*** *Armin D. Ebner, Lutfi Erden, Jason Ho*

4:35 Paper 628e: Limits of Rapid Pressure Swing Adsorption Processes: Does a Minimum Bed Size Factor Exist? — ***Aaron Moran***, *Orhan Talu*

4:55 Paper 628f: Thermal Modulation in High-Capacity Pressure Swing Adsorption via Incorporation of Microencapsulated Phase-Change Material — ***Stephen J. A. DeWitt***, *Héctor Octavio Rubiera Landa, Eli Carter, Jongwoo Park, Krista S. Walton, David S. Sholl, Yoshiaki Kawajiri, Matthew J. Realff, Ryan P. Lively*

5:15 Paper 628g: The Exact Equivalence Between Diffusion and LDF Models — ***Stefano Brandani***

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(629) Self-Assembly in Solution
Wednesday, Nov 1, 3:15 PM
MCC, M100B

Paschalis Alexandridis, Chair
Yakov Lapitsky, Co-Chair
Kenneth Mineart, Co-Chair

Sponsored by: Interfacial Phenomena

3:15 Paper 629a: Redox-Triggered Mixing and Demixing of Surfactants Within Assemblies Formed in Solution and at Surfaces — ***Nicholas L. Abbott***

3:30 Paper 629b: Static and Dynamic Signatures of Branching in Wormlike Micelles (WLMs) via Advanced Techniques in Rheology and Neutron Scattering — ***Michelle A. Calabrese***, *Simon A. Rogers, Lionel Porcar, Norman J. Wagner*

3:45 Paper 629c: Self-Assembly of Achiral Surfactants Can Conduct Enantioselective C-C Bond Formation of Amino Acid Derivative — ***Hiroshi Umakoshi***, *Fumihiko Iwasaki, Keishi Suga, Yukihiro Okamoto*

4:00 Paper 629d: A Statistical Associating Fluid Theory (SAFT) Framework for Aqueous Nonionic Surfactant Systems — ***Aubrey Winiarski***, *Arthur S. Gow*

4:15 Paper 629e: First Proof of Self-Assembly of Block Copolymers in a Deep Eutectic Solvent — ***Dannie J. G. P. van Osch***, *Marco M. R. M. Hendrix, Nicole M. W. van der Heijden, Jaap van Spronsen, A. Catarina C. Esteves, Remco Tuinier*

4:30 Paper 629f: Fast and Slow Dynamical Processes in Simulations of Block Copolymer Micelles — ***Joshua Mysona***, *David Morse, Alon McCormick*

4:45 Paper 629g: Synthesis of Hydrophobically Modified Polybetaines (HMPB) and Study of Their Self-Assembly by Molecular Dynamics Simulations — *Xiao Zhao, Ashwin Ravichandran, Sarkyt Kudaibergenov, Rajesh Khare,* ***Nurxat Nuraje***

5:00 Paper 629h: A Hexagonal Columnar Liquid Crystal–Phase Formation in Dilute Solutions of Carbon Nanotubes — ***Vida Jamali****, Francesca Mirri, Paul van der Schoot, Fred MacKintosh, Matteo Pasquali*

5:15 Paper 629i: Computational Phase Space Screening of Isotropic Multi-Well Pair Potentials — ***Julia Dshemuchadse****, Michael Engel, Pablo F. Damasceno, Carolyn L. Phillips, Sharon C. Glotzer*

5:30 Paper 629j: Methanol Self-Association and Preferential Solvation of Chelating Agents for the Extraction of Nuclear Fission Products in Supercritical CO_2 — ***Trent R. Graham****, Daniel J. Pope, Aurora E. Clark, Steven R. Saunders*

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(630) Stem Cells in Tissue Engineering
Wednesday, Nov 1, 3:15 PM
MCC, 208C/D

Ipsita Banerjee, Chair
Basak Uygun, Co-Chair

Sponsored by:
Engineering Fundamentals in Life Science

3:15 Paper 630a: Use of Adipocyte Stem Cells as a Surrogate Endothelium for Vascular Grafts — ***Robert Tranquillo***

3:55 Paper 630b: Engineering Islet-Specific Microvascular Network Within hPSC-Derived Pancreatic Islet Organoids — *Joseph E. Candiello, Taraka Sai Pavan Grandhi, Jacob Dale, Jason Beare, Suzanne Bertera, Kaushal Rege, Jay Hoying, Prashant N. Kumta,* ***Ipsita Banerjee***

4:13 Paper 630c: Modeling Diseased BBB Through Directed Differentiation of Patient-Derived iPSCs into Brain Microvascular Endothelial Cells — ***Hannah S. Seo****, Catherine A. A. Lee, Frank S. Bates, Jakub Tolar, Samira M. Azarin*

4:31 Paper 630d: hESC-Derived Striatal Cells Generated Using a Scalable 3D Hydrogel Promote Recovery in a Huntington's Disease Mouse Model — ***Maroof M. Adil****, David V. Schaffer*

4:49 Paper 630e: An Integrated Miniature Bioprocessing for Personalized Human Induced Pluripotent Stem Cell Expansion and Differentiation into Neural Stem Cells — ***Haishuang Lin****, Qiang Li, Yuguo Lei*

5:07 Paper 630f: Oligodendrocyte Precursor Cell Intracellular Redox State Is Dependent on 3D Hydrogel Properties — ***Lauren Russell****, Kyle Lampe*

5:25 Paper 630g: NANOG Restores the Myogenic Differentiation Potential of Senescent Myoblasts — ***Aref Shahini****, Debanik Choudhury, Mohammadnabi Asmani, Ruogang Zhao, Pedro Lei,* ***Stelios T. Andreadis***

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(631) Survey Results and Best Practices: Laboratory Instruction (Invited Talks)
Wednesday, Nov 1, 3:15 PM
MCC, 205C

Margot Vigeant, Co-Chair
Kevin Dahm, Co-Chair
David L. Silverstein, Co-Chair

Sponsored by:
Undergraduate Education

3:15 Introductory Remarks

3:20 Paper 631a: Laboratories in the Chemical Engineering Curriculum: Current State and Best Practices — ***Margot Vigeant****, Kevin Dahm, David L. Silverstein, Kevin Hadley*

3:50 Panel Discussion

4:50 Concluding Remarks

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(632) Thermophysics and Reactions in Energetic Materials
Wednesday, Nov 1, 3:15 PM
MCC, 200J

Lori J. Groven, Chair
Edward Dreizin, Co-Chair

Sponsored by: Energetics

3:15 Introductory Remarks

3:20 Paper 632a: Combustion of Mg-S and Zr-S Reactive Nanocomposite Powders Heated to Ignition at Different Rates — ***Ian Monk****, Mirko Schoenitz, Edward Dreizin*

3:37 Paper 632b: Effect of Flow Conditions on Burn Rates of Magnesium and Magnesium-Containing Reactive Material Particles — ***Xinhang Liu****, Song Wang, Mirko Schoenitz, Edward Dreizin*

3:54 Paper 632c: Quantitative Description of the Biocidal Effectiveness of Combustion Products of Iodine-Bearing Reactive Materials — ***Song Wang****, Mirko Schoenitz, Sergey A. Grinshpun, Edward Dreizin*

4:11 Paper 632d: Process Scale-Up for Production of Bis-Tetrazol-Amine and *N,N'*-Bis-(1*H*-tetrazol-5-yl)-Hydrazine — *Jonathan Lavoie,* ***Charles Dubois****, Catalin Florin Petre, Durand Simon*

4:28 Break

4:38 Paper 632e: Investigation of the Processability of Tetrazole Polyelectrolytes as Binders for Nitrogen-Rich Composite Propellants — ***Jean-Christophe St-Charles****, Charles Dubois*

4:55 Paper 632f: Tuning of Energetic Material Microwave Enhancement Through Micro/Nanostructure — ***Stuart J. Barkley****, Keke Zhu, Raymond Sucaet, Michael Thompson, James B. Michael, Travis R. Sippel*

5:12 Paper 632g: Burning Rate Control of Energetic Materials with Thermally Switchable Microwave Properties — ***Stuart J. Barkley****, Keke Zhu, Kyle Uhlenhake, James B. Michael, Travis R. Sippel*

5:29 Paper 632h: Field Switching of Monopropellant Burning Rate: Dielectrophoretic Control of Nitromethane Thermal Conductivity Using Field-Aligned Carbon Nanomaterials — ***Adam Lawrence****, Travis R. Sippel*

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(633) Upgrading Products of Thermal Deconstruction
Wednesday, Nov 1, 3:15 PM
MCC, 101I

Blake A. Simmons, Chair

Sponsored by:
Thermal Deconstruction of Biomass

3:15 Paper 633a: Fire-Adapted Microbes — ***Jonathan S. Schilling****, Jiwei Zang, Hunter Simpson, Claudia Schmidt-Dannert, Robert C. Brown*

3:40 Paper 633b: Rewiring Yeast to Improve Cellobiose Fermentation — ***Jamie H. D. Cate***

4:05 Paper 633c: Engineering Strategies for Improving Microbial Utilization of Thermally Depolymerized Biomass — ***Laura R. Jarboe****, Zhiyou Wen, Robert C. Brown, Kirsten Davis, Tao Jin*

4:30 Paper 633d: Production of Fermentation Substrates from Thermal Deconstruction of Lignocellulose — ***Marjorie Rover****, Patrick H. Hall, John Stanford, Ryan Smith, Robert C. Brown*

4:55 Paper 633e: Biological Conversion of Thermochemical Wastewater Streams — ***Gregg T. Beckham***

5:20 Paper 633f: Biological Processing of Anhydro Cellodextrins — ***Jake K. Lindstrom****, Peter N. Ciesielski, Ashutosh Mittal, Kirsten Davis, Haoqin Zhou, Zhiyou Wen, Laura R. Jarboe, Robert C. Brown*

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(634) USA-China Progress in Biomass Conversion Technologies II
Wednesday, Nov 1, 3:15 PM
MCC, 200E

Shijie Liu, Chair
Ronghou Liu, Co-Chair

Sponsored by:
Biorefinery Technologies for Forest-Based Lignocellulosic Biomass

3:15 Paper 634a: Lignin Aerobic Oxidation Catalyzed by Sn(IV) Using Dioxygen in Biphasic System — ***Chao Liu***

3:40 Paper 634b: A Novel Transport-Reaction Model for the Estimation of Topochemical Changes During the Pretreatment of Plant Biomass Using Raman Spectroscopy — ***Sahana Ramanna****, Bandaru V. Ramarao, Feng Xu, Shri Ramaswamy*

4:05 Paper 634c: Ex-Situ Catalytic Fast Pyrolysis of Biomass over HZSM-5 in a Two-Stage Fluidized-Bed/Fixed-Bed Combination Reactor — ***Changsong Hu***

4:30 Paper 634d: Engineering Innovative Polyelectrolyte Complex Membranes with Enhanced Pervaporation Performance in Ethanol Dehydration — ***Ziqiang Tong****, Xiufeng Liu, Baoquan Zhang**

4:55 Paper 634e: Biphasic Tandem Catalytic Process for Renewable Biofuel Production — ***Hongfei Lin***

5:20 Paper 634f: Nano Carbon Structures from Cellulosic Biomass for Use as Functional Materials — ***Jeffrey Wang****, Benjamin Frigo-Vaz, Ping Wang*

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(635) Water Treatment, Desalination, and Reuse III
Wednesday, Nov 1, 3:15 PM
MCC, M100H

Brian Chaplin, Co-Chair
Milad R. Esfahani, Co-Chair
Ngoc Bui, Co-Chair
Isabel Escobar, Co-Chair
Jamie Hestekin, Co-Chair

Sponsored by:
Membrane-Based Separations

3:15 Paper 635a: Towards the Control of Fouling Behavior of Hollow Fiber Membranes via High-Throughput Screening — ***Amir S. Kazemi****, Seung Mi Yoo, Raja Ghosh, David R. Latulippe*

3:35 Paper 635b: Influence of Backwashing on the Pore Size of Hollow Fiber Ultrafiltration Membranes — *Ebrahim Akhondi, Farhad Zamani, Adrian Law, William B. Krantz, Anthony G. Fane,* ***Jia Wei Chew***

3:55 Paper 635c: A Simple, Reactive Approach to Mitigate Fouling and Concentration Polarization in Reverse-Osmosis Systems — ***Manish Kumar****, Rajarshi Guha, Boya Xiong, Tevin Moore, Michael Geitner, Darrell Velegol*

4:15 Paper 635d: Graphene Oxide Membranes in Extreme Operating Environments: Concentration of Kraft Black Liquor — *Fereshteh Rashidi, Nikita Kevlich, Scott A. Sinquefield, Meisha Shofner,* ***Sankar Nair***

4:35 Paper 635e: Water Permeation Through Structural Defects of Single-Layered Graphene Oxide Membranes — ***Weiwei Xu***

4:55 Paper 635f: Braided-Reinforced Thin-Film Composite (TFC) Nanofiltration Hollow Fiber Membranes — *Lingling Xia,* ***Jeffrey McCutcheon***

5:15 Paper 635g: Naphthenic Acids Removal from High-TDS Produced Water by Persulfate-Mediated Iron Oxide-Functionalized Catalytic Membrane, and by Nanofiltration — *Ashish Aher, Andrew Colburn, Hongyi Wan,* ***Dibakar Bhattacharyya***

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(636) Workshop: Best Practices in Advising and Mentoring Undergraduate and Graduate Students
Wednesday, Nov 1, 3:15 PM
MCC, 205D

Lisa G. Bullard, Co-Chair
Taryn Bayles, Co-Chair
Katie Cadwell, Co-Chair

Sponsored by: Education

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(637) Rapid-Fire Session: Environmental Division
Wednesday, Nov 1, 4:45 PM
MCC, 102E

Debalina Sengupta, Chair

Sponsored by:
Environmental Division

4:45 Paper 637a: Effect of MnO_2 Catalyst and Electrode Geometry on Nonthermal Plasma Reactor Combined with Ceramic Filter for Trichloroethylene Decomposition — ***Yuta Yasuda****, Junichi Ida, Tatsushi Matsuyama, Hideo Yamamoto*

4:50 Paper 637b: Sustainability Assessment of Cement Manufacturing Processes Based on Emergy and Ecological Footprint Analysis — *Hrvoje Mikulčić,* ***Heriberto Cabezas****, Milan Vujanović, Neven Duić*

4:55 Paper 637c: A Bi-Dimensional Experimental Cell and Image Analysis: An Effective Device to Validate Model Predictions Applied to Electro-Transport of Heavy Metals — *Juan P. Barraza,* ***Rocio Tijaro-Rojas****, A. Nastasia Allred, Pedro E. Arce*

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(638) Poster Session: NH_3 Energy*
Wednesday, Nov 1, 6:00 PM
MCC, 101F/G

Sponsored by:
NH_3 Energy* — Enabling Optimized, Sustainable Energy and Agriculture

Paper 638a: Cheap Energy Production and Delivery Everywhere Including Mobile Applications — ***David Judbarovski***

Paper 638b: N_2 Reduction Electrocatalyst Surface Environment and Catalyst Studies for Ammonia Synthesis — ***Sergio I. P. Bakovic****, Mason J. Belue, Lauren F. Greenlee*

Paper 638c: Ammonia's Role in Enabling Widespread Renewable Power and Transport in Australia — ***Michael D. Dolan****, Louis Wibberley, Daniel Roberts, Brett Cooper*

Paper 638d: Auto-Ignition of a Non-Carbon Nitrogen-Based Monofuel — ***Bar Mosevitzky***

Paper 677f: Influence of H_2/N_2 Ratio on Dynamic Behavior of Ammonia Production on Ru Catalyst Under Low Pressure Condition — ***Hideyuki Matsumoto****, Javaid Rahat, Tetsuya Nanba*

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(639) Poster Session: Thermal Deconstruction
Wednesday, Nov 1, 6:00 PM
MCC, 101I

Jill Euken, Chair

Sponsored by: Thermal Deconstruction of Biomass

Paper 639a: Ionic Liquid Pretreatment of Lignocellulosic Biomass: Effect of Biomass Composition on Pretreatment Efficiency — ***Vasudha Kotia****, Vijayaraghavan Ranganathan, Vidhya Rangaswamy, Pavankumar Aduri, Antonio F. Patti, Douglas R. MacFarlane, Santosh B. Noronha*

Paper 639b: Enabling Microbial Utilization of Lignin-Derived Monomers — ***Kirsten Davis****, Marjorie R. Rover, Davinia Salvachua, Laura Jarboe, Gregg T. Beckham, Zhiyou Wen, Ryan G. Smith, Robert Brown, Xianglan Bai, Yuan Xue*

Paper 639c: Comparison of Product Distribution, Content and Fermentability of Biomass in a Hybrid Thermochemical/Biological Processing Platform — ***Zhanyou Chi****, Xuefei Zhao, Tannon J. Daugaard, Marjorie R. Rover, Patrick A. Johnston, Andre Salazar, Ryan G. Smith, Robert Brown, Zhiyou Wen, Olga Zabotina,* ***Laura Jarboe***

Paper 639d: Low-Temperature Hydrogenation of Pyrolytic Lignin over Ru/TiO_2: 2D HSQC and ^{13}C NMR Study of Reactants and Products — ***Daniel J. McClelland****, Wen Chen, Ali Azarpira, John Ralph, Zhongyang Luo, George W. Huber*

Paper 639e: One-Step Fermentable Sugar Production from Lignocellulosic Biomass via Soluble Magnesium Salt-Based Catalyst — *Xianni Qi, Yuanyuan Zhang,* ***Qinhong Wang****, Yanhe Ma*

Paper 639f: Selective Conversion of Ashe Juniper Waste into Levoglucosenone and Acetol — ***Julius Choi****, Sergio Capareda*

Paper 639g: Biofuel Precursor Solubilized Carbohydrates Production from Lignocellulosic Biomass Using Solvent Liquefaction — ***Arpa Ghosh****, Robert C. Brown*

Paper 639h: Pericyclic Reactions in Xylose Pyrolysis and Implications for Xylan Pyrolysis — ***Charles J. McGill****, Phillip R. Westmoreland*

Paper 639i: Analyzing the Torrefaction Products of Galactomannan and Its Monosaccharide Constituents — ***Arnab Bose,*** *Phillip R. Westmoreland*

Paper 639j: Thermal Deconstruction Opens Biomass for Acid Hydrolysis to Monosaccharides — ***Jake K. Lindstrom****, Peter N. Ciesielski, Chad Peterson, Juan Proano-Aviles, Preston A. Gable, Robert C. Brown*

Paper 639k: Conversion of Carboxylic Acids to Linear Olefins by Combined Hydrogenation/Dehydration Reactions — ***Jher Hau Yeap****, Bartosz Rozmysłowicz, Jeremy S. Luterbacher*

Paper 639l: Protection of Carbohydrates During Biomass Deconstruction Using Formaldehyde — ***Ydna M. Questell-Santiago****, Masoud Talebi Amiri, Li Shuai, Jeremy S. Luterbacher*

Paper 639m: Comprehensive Study of Pilot-Scale Fast Pyrolysis Data, 2015 to 2017 — ***Katherine R. Gaston****, Esther Wilcox*

Paper 639n: A Microkinetic Model for the Catalytic Upgrading of the Bio-Oil Model Compound Acetic Acid — ***Lauren Dellon****, Chun-Yi Sung, David Robichaud, Linda J. Broadbelt*

Paper 639o: Upgrading Fast-Hydropyrolysis Products of Cellulose to Higher-Molecular-Weight Products Using Systems-Level Molecular Mapping — ***Taufik Ridha****, Emre Gençer, Yiru Li, Mohit Tawarmalani, W. Nicholas Delgass, Fabio Ribeiro, Rakesh Agrawal*

Paper 639p: Converting Lignin to Value-Added Products with Copper-Doped Catalysts in Supercritical Methanol — ***Yu Gao****, Marcus Foston*

Paper 639q: Cleavage of Lignin Model Polymers with Copper-Doped Catalysts in Supercritical Methanol — ***Yu Gao****, Marcus Foston*

Paper 639r: Mechanistic Study of Guaiacol Fast Pyrolysis Using DFT Calculations, Microkinetic Model and Experiments — ***A. Yerrayya****, Upendra Natarajan, R. Vinu*

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(640) 2D Nanocomposites: New Composites with 2-Dimensional Nanomaterials
Thursday, Nov 2, 8:00 AM
MCC, 211D

Pingwei Liu, Chair
Evan K. Wujcik, Co-Chair
Vilas G. Pol, Co-Chair

Sponsored by: Composites

8:00 Paper 640a: Autoperforation of 2D Materials for Generating Two-Terminal Memresistor Janus Particles with Nonvolatile Memory — ***Pingwei Liu****, Albert Tianxiang Liu, Daichi Kozawa, Juyao Dong, Max Saccone, Volodymyr Koman, Song Wang, Minhao Wong, Michael Strano*

8:15 Paper 640b: Synthesis and Properties of Polymer/Graphene Oxide (GO) Thermosets with Multifunctional GO as a Crosslinker — ***Heonjoo Ha****, Jaesung Park, KiRyong Ha, Benny D. Freeman, Christopher J. Ellison*

8:30 Paper 640c: Polymer Silica Composite Nanofibers via Sol-Gel Electrospinning — ***Tahira Pirzada****, Sara A. Arvidson, Carl D. Saquing, S. Sakhawat Shah, Saad A. Khan*

8:45 Paper 640d: Graphene Oxide/Lipid Composite Material Towards a Multifunctional Drug Delivery Vehicle — ***Mohammad Shahadat Hussain Sarkar,*** *Md. Alamin Miraz, Ashiqur Rahman, Yang Lu, Vu Phan, Clayton S. Jeffryes, Evan K. Wujcik*

9:00 Paper 640e: Localizing Graphene at the Interface of HDPE/PLA Polymer Blends — ***Sung Cik Mun****, Min Jae Kim, Liangliang Gu, Monica Cobos, Christopher W. Macosko*

9:15 Paper 640f: Cocontinuous Ternary Polymer Nanocomposites with Interfacial Graphene Nanoplatelets — ***Llan Bai****, Radhika Sharma, Catherine Esnaashari, Christopher W. Macosko, Xiang Cheng*

9:30 Paper 640g: Investigating Catalytic Properties of $ReSe_2$ Edge and Basal Plane for Hydrogen Evolution Reaction — ***Zhenjing Liu****, Zhengtang Luo*

(641) Advances in Biocatalysis and Biosynthesis I: Cellular Engineering Applications

Thursday, Nov 2, 8:00 AM
MCC, 208C/D

Ryan Summers, Chair
Seok Hoon Hong, Co-Chair

Sponsored by: Bioengineering

8:00 Paper 641a: Pseudomonas sp. ADP Biofilms: Differentiation of Expression in Atrazine-Degrading Genes and Lectin Binding Analysis — ***Michael Delcau***, *Tonya L. Peeples*

8:18 Paper 641b: Biocatalytic Production of the High-Value Biochemical Paraxanthine from Caffeine — ***Shelby Brooks***, *Madeline Stewart, Ryan M. Summers*

8:36 Paper 641c: Combinatorial CRISPRi Expedites Microbial Metabolic Engineering — ***Brady F. Cress***, *Krystyna K. Farrell, Quentin D. Leitz, Robert J. Linhardt, Mattheos A. G. Koffas*

8:54 Paper 641d: Metabolic Engineering of Microorganisms for the Efficient Synthesis of Polysaccharides — ***Asher J. Williams***, *Wenqin He, Mattheos A. G. Koffas, Robert J. Linhardt*

9:12 Paper 641e: Metabolic Engineering for Bacterial Production of Caffeic Acid–Derived Phenethyl Esters and Amides in *Escherichia coli* — ***Jian Wang***, *Monika Mahajani, Shenieka Jackson, Yaping Yang, Eric Ferreira, Yuheng Lin, Yajun Yan*

9:30 Paper 641f: Rerouting Acetyl-CoA and NADPH to Improve Lipid and Oleochemical Production in Yarrowia lipolytica — ***Erqing Jin***, *Lynn Wong, Peng Xu*

9:48 Paper 641g: Engineering Biomolecular Scaffolds for Enhanced Biocatalysis — ***Wilfred Chen***

(642) Advances in Food and Bioprocess Engineering

Thursday, Nov 2, 8:00 AM
MCC, 206A/B

Nuttha Thongchul, Chair
Mei Shao, Co-Chair
Zhongqiang Wang, Co-Chair

Sponsored by: Food

8:00 Paper 642a: Challenges of Process Modeling in the Agrifood Industry — ***Spencer D. Schaber***

8:18 Paper 642b: Modeling and Optimization of Cholesterol Oxidase Production by Streptomyces olivaceus MTCC 6820 Using Response Surface Methodology Coupled with Artificial Neural Network-Genetic Algorithm — ***Shraddha Sahu***, *Shailendra Singh Shera,* ***Rathindra Mohan Banik***

8:36 Paper 642c: Effect of Different Short-Chain Carboxylic Acids on the Kinetics of Growth and Production of Natamycin by *Streptomyces natalensis* — ***Elsayed A. Elsayed***, *Mohamed A. Farid, Mohammad Wadaan, Hesham El-Enshasy*

8:54 Paper 642d: Prediction of Swelling Behavior of Cross-Linked Maize Starch Suspensions — *Prasuna Desam, Jinsha Li, Osvaldo Campanella,* ***Ganesan Narsimhan***

9:12 Paper 642e: Thermal and Rheological Characterization of Sugar Cane Honeys for the Modeling of Evaporation Systems — ***Angela Liliana Alarcón Rodríguez***, *Paulo Cesar Narváez Rincón, Alvaro Orjuela, Edgar Camilo Camacho Poveda*

9:30 Paper 642f: Selective Proteins Extractions from Biomass Using Pulsed Electric Field: Example of Macroalgae Ulva Processing — ***Alexander Golberg***, *Francois Fernand, Mark Polikovsky, Martin Sack, Georg Muller*

9:48 Paper 642g: (Keynote) Development of Bioprocess Platform for Cordycepin Production by *Cordyceps militaris* — ***Hesham El-Enshasy***, *Mohammad Soltani, Roslinda Abd Malek*

(643) Advances in Metabolic Engineering I: Emerging Tools and Techniques

Thursday, Nov 2, 8:00 AM
MCC, 207A/B

Thomas J. Mansell, Chair
Nikhil U. Nair, Co-Chair

Sponsored by: Bioengineering

8:00 Paper 643a: Selecting for Small Molecule Production in Competitive Microfluidic Droplets — *Jessica M. Velez,* ***Joshua K. Michener***

8:18 Paper 643b: Improving Glucaric Acid Production by Alleviating Oxidative Stress in *E. coli* — ***Lisa M. Guay***, *Kristala L. J. Prather*

8:36 Paper 643c: Investigation of Metabolite Channeling in Central Bacterial Pathways — ***Mary Abernathy***, *Lian He, Whitney D. Hollinshead, Yinjie Tang*

8:54 Paper 643d: Cell-Free Metabolic Engineering for Heterologous In-Vivo Pathway Optimization — ***Joseph Rollin***, *Christopher Johnson, Peter St. John, Gregg T. Beckham*

9:12 Paper 643e: Genetically Programmable Assembly of Microbial Communities for Enhanced Biosynthetic Efficiency — ***Bradley Silverman***, *Mark Kozlowski, David Tirrell*

9:30 Paper 643f: A Generic Strategy to Maintain Stable, Multi-Member Microbial Consortia — ***NaRae Lee***, *Jeremy Jie Ming Kwok, Xiaoqiang Ma, Liming Yang, Kang Zhou, Dong-Yup Lee*

9:48 Paper 643g: Advances in Metabolic Engineering I: Emerging Tools and Techniques (Featured Presentation) —

(644) Advances in Shale Characterization and Fluids Management

Thursday, Nov 2, 8:00 AM
MCC, 200C

Jared Ciferno, Chair
Rameshwar Srivastava, Co-Chair
Jason Trembly, Co-Chair
David Cercone, Co-Chair

Sponsored by:
Advances in Fossil Energy R&D

8:00 Paper 644a: Enhancing Unconventional Shale Porosity and Permeability by Subcritical Water Treatment — ***Md. Rifat Hasan***, *M. Toufiq Reza, Julie Sheets, David R. Cole*

8:22 Paper 644b: Research to Investigate the Potential for Enhanced Oil Recovery in the Bakken Petroleum System — ***James A. Sorensen***, *Steve Hawthorne, Bethany Kurz, Lawrence Pekot, Steve Smith, Lu Jin, Charles D. Gorecki, Edward N. Steadman, John A. Harju*

8:44 Paper 644c: Evaluation of Reinjection as a Means to Increase Petroleum Production from the Utica/Point Pleasant Unconventional Play: Impact of Reinjection Fluid Composition, Pressure, and Pore Size on Hydrocarbon Bubble Point Behavior — ***Michael Spencer***, *Ravinder Garlapalli, Jason Trembly*

9:06 Paper 644d: Chemical Controls on Secondary Mineral Precipitation of Fe and Ba in Hydraulic Fracturing Systems — ***Adam D. Jew***, *Qingyun Li, Megan Dustin, Anna Harrison, Claresta Joe-Wong, Dana Thomas, Kate Maher, Gordon Brown Jr., John Bargar*

9:28 Paper 644e: Advanced Supercritical Water-Based Process Concepts for Treatment and Beneficial Reuse of Produced Water Generated by Oil/Gas Production — ***Jason Trembly***, *David Ogden*

9:50 Paper 644f: Liquid CO_2-in-Mineral Oil Emulsions Stabilized by Siloxane–Long-Chain Alkyl Surfactants and Application as a Waterless Hydraulic Fracturing Fluid — ***Shehab Alzobaidi,*** *Jason J. Lee, Summer Jiries, Eric J. Beckman, Gianfranco Rodriguez, Robert J. Perry, Keith P. Johnston, Robert Enick*

10:12 Paper 644g: Laser-Induced Breakdown Spectroscopy (LIBS): A Potential Technique for In-Situ Geochemical Characterization of Unconventional Shales — ***Jinesh Jain***, *Derrick Quarles Jr., Johnathan Moore, Dustin McIntyre, Dustin Crandall*

(645) Alternative Fuels

Thursday, Nov 2, 8:00 AM
MCC, L100C

Hsi-Wu Wong, Chair
Richard H. West, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

8:00 Paper 645a: Highly Selective FT Synthesis for Production of JP-8 Jet Fuel from Coal and Coal/Biomass Mixtures — ***Andrew Lucero***, *Brittany Koob, Brandon Cline, Patrick Woolcock, Curtis Thompson, Kevin McCabe*

8:22 Paper 645b: Microfibrous Entrapped Catalyst Structure for Highly Exothermic Reaction: Fischer-Tropsch Synthesis — ***Xinquan Cheng***, *Bruce Tatarchuk*

8:44 Paper 645c: Hydrogen Production from Thermal and Catalytic Gasification of Biomass in a Fluidized CREC-Riser Simulator: Thermodynamic Modeling and Experimental Results — ***Benito Serrano Rosales***, *Hugo de Lasa, Jahirul Mazumder, Blanca Flor Orozco Salazar, Jose Ramses Garcia Elias, Ana Giron S.*

9:06 Paper 645d: A Generalized Kinetic Model for Transesterification and Saponification — ***Pulkit Chhabra***, *Sebastian Mosbach, Markus Kraft, Iftekhar A. Karimi*

9:28 Paper 645e: Microwave-Assisted Co-Pyrolysis of High-Ash Indian Coal and Rice Husk and Detailed Product Characterization — ***Rajasekhar Reddy Busigari***, *R. Vinu*

9:50 Paper 645f: Highly Selective Catalytic Conversion of Furfural to γ-Butyrolactone — ***Tiefeng Wang***, *Xiaodan Li, Yafei Li*

10:12 Paper 645g: In-Situ Drifts Studies over Cobalt Catalyst for Hydrogen Production from Ethanol — ***Anand Kumar***, *Anchu Ashok, Md. Abdul Matin, Faris Tarlochan*

(646) Big Data in Process Modeling, Estimation and Control

Thursday, Nov 2, 8:00 AM
MCC, 103F

Ravendra Singh, Chair
Matthew J. Realff, Co-Chair

Sponsored by:
Data and Information Systems

8:00 Paper 646a: Pipeline Big Data Analysis: Leak Localization — ***Stevan Dubljevic***, *Xiaodong Xu*

8:17 Paper 646b: Big Data Approach to Fault Detection, Diagnosis and Maintenance Optimization in Batch Processes — ***Melis Onel***, *Chris A. Kieslich, Yannis A. Guzman, Efstratios N. Pistikopoulos*

8:34 Paper 646c: An Information Entropy-Based Criterion for Variable Selection Performance Assessment — ***Q. Peter He***, *Kerul Suthar, Jangown Lee*

8:51 Paper 646d: Health Monitoring of Multiscale Systems Using an Optimal Multi-Rate Wireless Sensor Network — ***Qiao Huang***, *Debangsu Bhattacharyya, Edward Sablosky, Katarzyna Sabolsky, Rajalekshmi Pillai*

9:08 Paper 646e: Learning-Based Automated Identification of Nuisance and Correlated Alarms — *Neha Goyal,* ***Yash Puranik***, *Alexander B. Smith, Bijan Sayyar-Rodsari*

9:25 Paper 646f: Dynamic Latent Variable Regression for Data Modeling and Monitoring — *Qinqin Zhu,* ***S. Joe Qin***

9:42 Paper 646g: Bayesian Model Averaging for Estimating the Spatial Temperature Distribution in a Steam Methane Reformer — ***Anh Tran***, *Marquis Crose, Andres Aguirre, Yangyao Ding, Madeleine Pont, Helen Durand, Panagiotis D. Christofides*

9:59 Paper 646h: Adaptive ARX Models for Non-Linear Chemical Processes: An Industrial Application — ***Zhenyu Wang***, *Suyash Singh, Ali Esmaili*

10:16 Paper 646i: Performance Evaluation of Anomaly Diagnosis System Based on Adaptive Resonance Theory — ***Yoshinari Hori***, *Yoshiharu Hayashi, Takaaki Sekiai, Hiroki Yamamoto, Shinji Hasebe*

(647) Biomaterials for Drug Delivery III: Scaffolds-Based Drug Delivery

Thursday, Nov 2, 8:00 AM
MCC, 210A/B

Timothy Brenza, Chair
Stephanie Christau, Co-Chair

Sponsored by: Biomaterials

8:00 Paper 647a: PEG Hydrogels with Tunable Biodegradation Rate for Sustained Delivery of Platelet-Rich Plasma for Treatment of Osteoarthritis — *Era Jain, Saahil Sheth, Nobuaki Chinzei, Natasha Case, Linda Sandell, Scott A. Sell, Muhammad Rai,* ***Silviya P. Zustiak***

8:18 Paper 647b: Control over the Temporal Profile and Sequence of Anticancer Therapeutics from Magnetically Responsive Hydrogels — ***Tania Emi***, *Tanner Barnes, Emma Orton, Anne Reisch, Zachary Silveira, Miranda Mitchell, Celia Dunn, Anita E. Tolouei, Stephen Kennedy*

8:36 Paper 647c: Electrospun Gelatin Nanofibers as Carrier for Controlled and Sustained Release of a Hydrophobic Drug — *Anindita Laha,* ***Chandra Sharma***, *Saptarshi Majumdar*

8:54 Paper 647d: Engineering of Degradable Biopolymer Films Loaded with Imiquimod for Controlled Release in a Mucosal Environment — *Lucas Garcia Camargo, Gabriela Souza Rezende, Stephany di Carla Santos, Michelle Franz Montan Braga Leite, Renata Nishida Goto, Andréia Machado Leopoldino,* ***Ângela Maria Moraes***

9:12 Paper 647e: Microparticles for the Delivery of Anti-Diabetic Drugs to the Adipose Tissue — ***Christopher Isely***, *Michael Hendley, Kendall Murphy, Prakasam Annamalai, Michael Gower*

9:30 Paper 647f: Template-Assisted Micro-Patterned Electrospun Nanofibrous Mat as a Potential Carrier for Controlled Drug Release — *Manohar Kakunuri, Mudrika Khandelwal,* ***Chandra S. Sharma***, *Stephen Eichhorn*

9:48 Paper 647g: PAG-Based Nanocomposite Hydrogels: Thermoresponsive Sol-Gel Transitions and Decomposition Rates Regulated by the LA/GA Ratio of PLGA-PAG-PLGA — ***Midori Kitagawa***, *Tomoki Maeda, Atsushi Hotta*

10:06 Paper 647h: Nanostructured Polymer Monoliths for Biomedical Applications — ***Yihui Xie***, *Marc A. Hillmyer*

(648) Biomaterials I: Instructive and Responsive Biomaterials

Thursday, Nov 2, 8:00 AM
MCC, 211A

Samira M. Azarin, Chair
Hongyan Ma, Co-Chair
Era Jain, Co-Chair

Sponsored by: Biomaterials

8:00 Paper 648a: Directing Immune Tolerance Using Quantum Dots to Control Self-Antigen Display and Stop Autoimmunity — *Krystina Hess,* ***Christopher M. Jewell***

8:18 Paper 648b: Electrospun Collagen Scaffold for Peripheric Nerve Regeneration — ***Carol Rivera Martinez***, *Janet Mendez, Jorge Almodovar*

8:36 Paper 648c: 3D Printing of Nerve Guidance Channels for Peripheral Nerve Repair — ***Wei Wu***

8:54 Paper 648d: Combined Physical and Biochemical Cues Direct the Growth of Inner Ear Neurites — ***Braden Leigh***, *Kristy Troung, Reid Bartholomew, Marlan Hansen, C. Allan Guymon*

9:12 Paper 648e: Harnessing Multi-Functional Microbial Cells for Designing Sweat-Responsive Bio-Hybrid Wearables — ***Wen Wang***, *Lining Yao, Chin-Yi Cheng, Teng Zhang, Hiroshi Atsumi, Luda Wang, Guanyun Wang, Oksana Anilionyte, Helene Steiner, Jifei Ou, Kang Zhou, Chris Wawrousek, Katherine Petrecca, Angela M. Belcher, Rohit Karnik, Daniel I. C. Wang, Xuanhe Zhao, Hiroshi Ishii*

9:30 Paper 648f: Development of Silk Protein Conjugates for Mucoadhesive Applications — *Danielle L. Heichel,* ***Kelly A. Burke***

9:48 Paper 648g: Laser-Activated Sealants for Skin Tissue Repair — ***Russell Urie***, *Deepanjan Ghosh, Mitzi Thelakkaden, Chengchen Guo, Jeff Yarger, Jacquelyn Kilbourne, Kaushal Rege*

10:06 Paper 648h: Layer-by-Layer Assembled Thin-Film Biomaterials as Porous Biomolecular Delivery Systems — *Adeline Gand, Mathilde Hindie, Michel Boissiere, Emmanuel Pauthe,* ***Paul R. Van Tassel***

(649) Biomolecular Engineering

Thursday, Nov 2, 8:00 AM
MCC, 208B

Benjamin J. Hackel, Chair
Tamara L. Kinzer-Ursem, Co-Chair
Adam Melvin, Co-Chair

Sponsored by:
Engineering Fundamentals in Life Science

8:00 Paper 649a: Protease-Responsive Droplets Engineered from Self-Assembled Disordered Proteins — ***Benjamin S. Schuster***, *Ellen H. Reed, Matthew C. Good, Daniel A. Hammer*

8:18 Paper 649b: Engineering Anti-EGFR Fibronectin Nanorings for Cancer Immunotherapy — ***Özgün Kılıç***, *Carston R. Wagner*

8:36 Paper 649c: Engineered Protein-Polymer Conjugates for Drug Delivery to the Central Nervous System — *Eugenie Jumai'an, Analia Vazquez Cegla, Natalie D. Smith, Allison Sirois, Maren E. Buck,* ***Sarah J. Moore***

8:54 Paper 649d: Covalent Heterobivalent Inhibitors for Drug Allergies — ***Peter Deak***, *Baksun Kim, Maura Vrabel, Byunghee Koh, Mark Kaplan, Tanyel Kiziltepe, Basar Bilgicer*

9:12 Paper 649e: Exploring the HIV V1V2 Loop Conformational Landscape with Protein Engineering — ***Jennifer Lai***, *Deeptak Verma, Chris Bailey-Kellogg, Margaret E. Ackerman*

9:30 Paper 649f: A Small Peptide Localizes to a Distinct Region of the Cell Membrane by Sensing Curvature — ***Edward Y. Kim***, *Erin Tyndall, Kerwyn Casey Huang, Fang Tian, Kumaran Ramamurthi*

9:48 Paper 649g: Technical Presentation — ***Hadley D. Sikes***

(650) Catalysis for C1 Chemistry: CO_2 Conversion and Methane Reforming

Thursday, Nov 2, 8:00 AM
MCC, L100D

Praveen Bollini, Chair
Basudeb Saha, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

8:00 Paper 650a: Towards the Design of Sulfur-Tolerant CO_2-Reforming Catalysts — ***Kerry M. Dooley***, *Changyi Jiang, Michael Janik, Bo Li, Jaren Lee*

8:18 Paper 650b: Development of Catalytic Process for CO_2 Utilization — ***Hongfei Lin***

8:36 Paper 650c: Catalytic Methanation of Carbon Dioxide with Ni/MgO Catalyst in Dual-Step Reductive Calcination — *Susanne Lux, Georg Baldauf-Sommerbauer,* ***Matthaeus Siebenhofer***

8:54 Paper 650d: Glycerol Transfer Hydrogenation of CO_2 Using Ir and Ru Carbene Organometallics Immobilized on Active Hydrotalcites in a Packed-Bed Flow Reactor — ***Jacob Heltzel****, Adelina Voutchkova-Kostal, Matthew Finn*

9:12 Paper 650e: Combining CO_2 Reduction with Propane Oxidative Dehydrogenation over Bimetallic Catalysts — ***Elaine Gomez****, Jingguang G. Chen*

9:30 Paper 650f: CO_2 Splitting Using MIEC Membranes — ***Xiao-Yu Wu****, Ahmed F. Ghoniem*

9:48 Paper 650g: Molten Metal Catalysts for Methane Pyrolysis — ***D. Chester Upham****, Alexi Khechfe, Zachary Snodgrass, Michael Gordon, Horia Metiu, Eric W. McFarland*

10:06 Paper 650h: Increasing Activity, Reducing Coking, and Promoting Unexpected Reaction Pathways During Methane Steam Reforming by Applying Uniform Electric Fields in a Scalable Reactor — ***Jake T. Gray****, Fanglin Che, Jean-Sabin McEwen, Su Ha*

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(651) Catalytic Hydrocarbon Processing I
Thursday, Nov 2, 8:00 AM
MCC, L100B

Steven Crossley, Chair
Nan Yi, Co-Chair
William W. Lonergan, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

8:00 Paper 651a: Oxidative Dehydrogenation of Propane Using CO_2 over Molybdenum Oxycarbidic Catalysts — ***Mark Sullivan****, Aditya Bhan*

8:20 Paper 651b: Alkali Promoted Mg_6MnO_8 Redox-Catalysts for Chemical Looping–Oxidative Dehydrogenation of Ethane: Mechanistic Investigations — ***Luke Neal****, Seif Yusuf, Vasudev Pralhad Haribal, Fanxing Li*

8:40 Paper 651c: Propane Dehydrogenation on MOF-Derived Iron Carbide Catalysts — ***Michele L. Sarazen****, Christopher W. Jones*

9:00 Paper 651d: Selective Oxidative Dehydrogenation of Propane to Propylene Using Boron Nitride Catalysts — ***Joseph Grant****, Carlos A. Carrero, Florian Göltl, Juan Venegas, Philipp Müller, Samuel P. Burt, Sarah Specht, William McDermott, Alessandro Chieregato, Ive Hermans*

9:20 Paper 651e: Pt-Fe Intermetallic Alloy Nanoparticles as Selective Propane Dehydrogenation Catalysts — ***Evan C. Wegener****, John E. Copple, Zhenwei Wu, Jeffrey T. Miller*

9:40 Paper 651f: Investigating the Role of Molybdenum During the Direct Conversion of Methane to Liquids Under Non-Oxidative Conditions — ***Vaidheeshwar Ramasubramanian****, Hema Ramsurn*

10:00 Paper 651g: Catalytic Consequences of Isolated and Paired Acid Sites in CHA Zeolites on Monomolecular Propane Cracking — ***Philip M. Kester****, John R. Di Iorio, Rajamani Gounder*

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(652) Chemical Modifications and Processing of Biomaterials
Thursday, Nov 2, 8:00 AM
MCC, 200D

Zhaohui Tong, Chair
Yulin Deng, Co-Chair

Sponsored by:
Forest and Plant Bioproducts Division

8:00 Paper 652a: Selective Lignin, Cellulose, and Hemicellulose Dissolution in Deep Eutectic Solvents — *Joan G. Lynam,* ***Narendra Kumar****, Mark Wong*

8:25 Paper 652b: Assessing the Dispersion Influence of Cellulose Nanofibers on Papermaking Applications — *Ana Balea, Cristina Campano, Noemi Merayo,* ***Angeles Blanco****, Carlos Negro*

8:50 Paper 652c: Fabrication of Functionalized Aerogels from Cellulose and Whole Biomass for Absorbing Formaldehyde from Indoor Air — ***Yang Liao****, Xuejun Pan*

9:15 Paper 652d: Cellulose-Based Injectable Hydrogel Composite for pH-Responsive Drug Delivery — ***Zhaohui Tong****, Nusheng Chen, Wilfred Vermerris, Ling Chen*

9:40 Paper 652e: Biodegradable Seed Wraps for Sustained Release of Pesticides for Crop Protection in Sub-Saharan Africa — ***Tahira Pirzada****, Abdus Salam, Nancy Vogel, Reny Mathew, Richard H. Guenther, Tim L. Sit, Med Byrd, Lokendra Pal, Charles H. Opperman, Saad A. Khan*

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(653) Circulating Fluidized Beds and Measurement Techniques in Fluid-Particle Systems
Thursday, Nov 2, 8:00 AM
MCC, 200I

Michael J. Molnar, Chair
Atish Kataria, Co-Chair

Sponsored by:
Fluidization and Fluid-Particle Systems

8:00 Paper 653a: Numerical Simulation and Experimental Study of a Micro Circulating Fluidized Bed — ***Yupeng Xu****, Jordan Musser, Tingwen Li, William A. Rogers, Balaji Gopalan, Greggory Breault, Jonathan Tucker, Rupen Panday*

8:18 Paper 653b: Attrition Prediction and Reactive Jet Cup Testing of Oxygen Carriers for Chemical-Looping Combustion — ***Nathan Galinsky****, Samuel Bayham, Ronald W. Breault*

8:36 Paper 653c: The Effect of Particle Shape on the Behavior of Group A Particles in Dilute Risers — ***Casey Q. LaMarche****, Peiyuan Liu, Kevin M. Kellogg, Christine M. Hrenya*

8:54 Paper 653d: Experimental Analysis of a Vortexing CFB for Process Intensification via High-G Flows — ***Michael Bobek****, Justin Weber, Jingsi Yang, Franklin D. Shaffer, Ronald W. Breault*

9:12 Paper 653e: Experimental Investigation of Horizontal Air Jets in Semi-Circular, Gas-Solid Fluidized Bed — *William Fullmer, Casey Q. LaMarche, Peiyuan Liu, Allan Issangya, Rasa Kales,* ***Ray Cocco****, Christine M. Hrenya*

9:30 Paper 653f: On the Euler-Lagrange Simulations of a Pilot-Scale Circulating Fluidized Bed Riser: Experimental Unit CFD-Based Design, Flow Structures and Particle Forces Analysis — ***Jonathan Utzig****, Waldir Pedro Martignoni, Francisco J. Souza, Henry F. Meier*

9:48 Paper 653g: Particle Phase Behavior Experimental Analysis on a Pilot-Scale CFB Riser Using Phase Doppler Anemometry — ***Jonathan Utzig****, Waldir Pedro Martignoni, Francisco J. Souza, Henry F. Meier*

10:06 Paper 653h: Non-Intrusive Characterisation of Particle Cluster Behaviours in a Riser Through Electrostatic and Vibration Sensing — ***Jingyuan Sun****, Yong Yan*

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(654) Colloidal Dispersions
Thursday, Nov 2, 8:00 AM
MCC, M100A

Ubaldo M. Córdova-Figueroa, Chair
Yoonjee Park, Co-Chair
Michael P. Tate, Co-Chair
Christina Tang, Co-Chair

Sponsored by:
Interfacial Phenomena

8:00 Welcoming Remarks

8:03 Paper 654a: Effect of Salt Concentration on the Ability to Form Stable Close-Packed Vesicular Dispersions for Stabilizing Suspensions of Dense Particles Against Sedimentation — *An-Hsuan Hsieh,* ***Yung-Jih Yang****, David S. Corti, Elias I. Franses*

8:19 Paper 654b: Toward a Better Understanding of Nanoassembly: Importance of Molecular Granularity on Colloidal Forces — ***Jaehun Chun****, Christopher J. Mundy, Gregory K. Schenter, Dongsheng Li, James J. De Yoreo*

8:35 Paper 654c: Structural Insights into DNA-Stabilized Silver Clusters Through Analytical Ultracentrifugation — *Danielle Schultz, Nancy J. Lin,* ***Jeffrey A. Fagan***

8:51 Paper 654d: Stabilization of Colloidal Suspensions with a Bimodal Distribution of Microparticles and Nanoparticles — ***Marzieh Moradi****, Stuart J. Williams, Gerold A. Willing*

9:07 Paper 654e: Rheological and Electrical Percolation Behavior of Carbon Black Suspensions in Polar Aprotic Solvents — *Norman Wagner,* ***Jeffrey J. Richards****, Paul Butler*

9:23 Paper 654f: Functional Hybrids Based on Assembly of 2D Materials and Polymeric Nanoparticles — ***Nader Taheri Qazvini****, Kylie Zane, Brian Schwartz, Matthew V. Tirrell, Juan de Pablo*

9:39 Paper 654g: Convective Fluid Motions in Droplets Driven by Global and Local Chemical Gradients — ***Nan Shi****, Todd M. Squires*

9:55 Paper 654h: Characterizing Gelatin Hydrogel Viscoelasticity with Diffusing Colloidal Probe Microscopy — ***Soheila Shabaniverki****, Jaime Juárez*

10:11 Paper 654i: Self-Immobilized Cross-Linked Enzyme Aggregates for Biocatalysis — ***Yang Kun-Lin****, Le Truc Nguyen*

10:27 Concluding Remarks

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(655) Community-Based Water Treatment Innovations
Thursday, Nov 2, 8:00 AM
MCC, 102F

Leslie M. Shor, Chair
Andi Rahardianto, Co-Chair

Sponsored by: Water

8:00 Paper 655a: Application of Semi-Batch Reverse-Osmosis (RO) Operation for Water Purification in Small Communities — ***Tae Lee****, Yoram Cohen, Anditya Rahardianto*

8:22 Paper 655b: EWB-Ecuador/USFQ Project: Contaminant Removal from Effluents Through the Use of Moringa oleifera Seeds for Application in Ecuadorian Rural Communities — *Andrés S. Lagos, Marlon M. Pico, Esteban R. Nuñez, Alina L. Trávez, M. Fatme Troya, Israel Sornoza, Juan S. Villarreal, José C. Andrade, Aldo J. Cunalata, Felipe D. Bastidas, Michel E. Vargas-Vallejo,* ***Andrea C. Landázuri****, Mario Caviedes*

8:44 Paper 655c: Performance of A-Stage Process Treating Wastewater Containing Domestic Food Waste from Disposers: An Alternative for Community-Based Sewage Treatment — ***Carlos Zamalloa****, Bo Hu*

9:06 Paper 655d: Artificial Intelligence for Organochlorine Pesticides Removal from Aqueous Solutions Using Entrapped NZVI in Alginate Biopolymer — *Ahmed S. Mahmoud, Rasha A. SaryEl-deen,* ***Mohamed K. Mostafa***

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(656) Computational Catalysis IV: Biomass Chemistry and Chemicals Production
Thursday, Nov 2, 8:00 AM
MCC, L100E

Heather Mayes, Chair
Samir H. Mushrif, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

8:00 Paper 656a: Developing Multiscale Models of Bimetallic Catalysts for the Hydrodeoxygenation of Bio-Oil Compounds — *Breanna Wong, Greg Collinge, Alyssa Hensley, Yong Wang,* ***Jean-Sabin McEwen***

8:18 Paper 656b: Mechanistic Insights into Hydrodeoxygenation of Phenol on Bimetallic Phosphide Catalyst — *Varsha Jain, Anna Taconi, Alicia Brown,* ***Neeraj Rai***

8:36 Paper 656c: Acylation of Furans in Acidic Zeolites: A DFT Study — ***Zhiqiang Zhang****, Maura Koehle, Raul F. Lobo, Stavros Caratzoulas, Dion G. Vlachos*

8:54 Paper 656d: Catalytic Conversion of Furfural to Methylfuran: Investigating Reaction Mechanisms on Ni and the Effect of Boron Doping on the Activity and Selectivity of the Catalyst — ***Arghya Banerjee****, Samir H. Mushrif*

9:12 Paper 656e: First-Principles Insights into the Mechanisms and Sites for Base-Catalyzed Aldol Condensation and Esterification over Copper — ***Ashwin Chemburkar****, Zhiyuan Tao, David D. Hibbitts, Enrique Iglesia, Matthew Neurock*

9:30 Paper 656f: Advancing the Selective Oxidation of Ethylene Glycol via Combining Novel Catalyst Design and Density Functional Theory (DFT) Calculations — ***Honghong Shi****,* ***Tuhin Suvra Khan****, R. V. Chaudhari, M. Ali Haider, Bala Subramaniam*

9:48 Paper 656g: Quantum Chemical Characterization of Catalytic Ester Decarbonylation: Olefins from Biomass — ***Büşra Dereli****, Manuel Ortuño, Christopher Cramer*

10:06 Paper 656h: Multiscale Models of Oxygen on Iron-Based Hydrodeoxygenation Catalysts: Elucidating the Effect of External Electric Fields and Surface Dopants — ***Jacob Bray****, Greg Collinge, Yong Wang, Catherine Stampfl, Jean-Sabin McEwen*

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(657) Critical Quality Attribute Monitoring and Control in Pharmaceutical Manufacturing I
Thursday, Nov 2, 8:00 AM
MCC, 205C

Huiquan Wu, Chair
Otute Akiti, Co-Chair

Sponsored by:
Pharmaceutical Discovery, Development and Manufacturing Forum

8:00 Paper 657a: Prediction of Tablet Dissolution by Process Parameters in Continuous Manufacturing — ***Golshid Keyvan****, Yifan Wang, Fernando Muzzio*

8:25 Paper 657b: Integrating Sensors for Monitoring Blend Content in a Pharmaceutical Continuous Manufacturing Plant — ***Savitha Panikar****, Jingzhe Li, Varsha Rane, Sean Gilliam, Gerardo Callegari, Bogdan Kurtyka, Sau Lee, Fernando J. Muzzio*

8:50 Paper 657c: Scientific and Regulatory Considerations for Developing the Control Strategy of a Continuous Manufacturing Process — ***Ying Zhang***

9:15 Paper 657d: Uncertainty Quantification and Global Sensitivity Analysis of Drug Delivery Primary Containers to Understand Process Capability and Key Risk Factors — *Fabrice Schlegel,* ***Pablo A. Rolandi***

9:40 Paper 657e: Nucleation Behavior of Eszopiclone-Butyl Acetate Solutions from Metastable Zone Widths — *Junbo Gong, Jingkang Wang,* ***Shijie Xu***

10:05 Paper 657f: Development, Implementation, and Use of an On-Line Laser Diffraction Particle Size Method in a Spray-Drying Manufacturing Process — ***Martin Warman****, Alon Vaisman*

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(658) Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains I
Thursday, Nov 2, 8:00 AM
MCC, 101E

Fengqi You, Chair
Debalina Sengupta, Co-Chair
Gerardo J. Ruiz-Mercado, Co-Chair

Sponsored by: Sustainable Energy

8:00 Paper 658a: Design of CO_2 Conversion to Dimethyl Carbonate by the Process-to-Planet Multiscale Modeling Framework — ***Kyuha Lee****, Bhavik R. Bakshi*

8:22 Paper 658b: Optimal Design of Biomass Supply Chain for Deploying Bioenergy with CCS (BECCS) in the UK — ***Di Zhang****, Niall Mac Dowell*

8:44 Paper 658c: Water Management Within Energy Systems — ***Omar J. Guerra****, G. V. Reklaitis*

9:06 Paper 658d: Considering Ecosystem Services in US Bioenergy Supply Chains — ***Daniel Garcia****, Fengqi You*

9:28 Paper 658e: Robust Multi-Period and Multi-Objective Strategic Planning of Hydrogen Networks — ***Gerald S. Ogumerem****, William W. Tso, C. Doga Demirhan, Changkyu Kim, Efstratios N. Pistikopoulos*

9:50 Paper 658f: A Stochastic Techno-Economic Model for Quantifying the Economic Costs of Cellulosic Bioenergy Pathways in the Northeast U.S. — ***Tristan Brown***

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(659) Developments in Biorefineries
Thursday, Nov 2, 8:00 AM
MCC, 101B

Eric C. D. Tan, Chair
Peyman Fasahati, Co-Chair
Kok Siew Ng, Co-Chair

Sponsored by:
Sustainable Biorefineries

8:00 Paper 659a: Commercial Biobutanol Production — ***Edward T. Davies***

8:25 Paper 659b: Techno-Economic Comparison of an Industrial-Scale Pyrolysis of Seaweed for Liquid Fuel Production: H_2 Production vs. H_2 Purchase Scenarios — ***Boris Brigljevic****, J. Jay Liu, Hee-Chul Woo*

8:50 Paper 659c: Techno-Economic and Life-Cycle Analysis for the Production of Renewable Acrylonitrile from Non-Food Biomass — ***Jadid Samad****, William Grieco, Amit Goyal*

9:15 Paper 659d: Relative Sustainability of Natural Gas-Assisted High-Octane Gasoline Blendstock Production from Biomass — ***Eric C. D. Tan****, Hao Cai, Michael Talmadge*

9:40 Paper 659e: In-Situ Catalytic Fast Pyrolysis of Nannochloropsis sp. Using Co-Mo Catalysts for Value-Added Chemicals — ***Ribhu Gautam****, R. Vinu*

10:05 Paper 659f: Wood Adhesive as a Coproduct of Cellulosic Alcohol: Crosslinking and Bond Performance — ***Islam Hafez****, Han-Seung Yang, Feng Jin Liew, Jonathan Schilling, William T. Y. Tze*

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(660) Experimental Methods in Adsorption
Thursday, Nov 2, 8:00 AM
MCC, M100D

Roger D. Whitley, Chair
Enzo Mangano, Co-Chair

Sponsored by:
Adsorption and Ion Exchange

8:00 Welcoming Remarks

8:05 Paper 660a: Measuring 3D Gas Adsorption Isotherms by X-Ray Computed Tomography — ***Lisa Joss****, Ronny Pini*

8:25 Paper 660b: Measurement of Water Adsorption Equilibrium and Kinetics Using the ZLC Technique — ***Alessio Centineo****, Stefano Brandani*

8:45 Paper 660c: Novel Approach for Kinetic Measurements for Low-Capacity Adsorbents — ***Enzo Mangano****, Mohammad A. Kalbassi, Roger D. Whitley, Stefano Brandani*

9:05 Paper 660d: Vibrational Gravimetric Analysis of Capillary Condensation of Propane in Nanoporous Rock — ***Younki Cho****, Ryan Lo, Keerthana Krishnan, Xiaolong Yin*

9:25 Paper 660e: Determination of Anthracene, Phenanthrene and Carbazole in Crude Anthracene by Capillary GC — *Liu Wei, Jiang Su-yu, Dan Zhang,* ***Li Hui-ping***

9:45 Paper 660f: Characterization of Chitosan Hydrogel with Improved Acid Stability Switched On by Carbon Dioxide — ***Le Quang Huy***, *Dimas Ardiyanta, Yusuke Shimoyama*

10:05 Paper 660g: Multiscale Modeling of the Breakthrough Behavior of Adsorption Columns — ***Gerassimos Orkoulas***, *Dipendu Saha*

10:25 Concluding Remarks

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(661) Fundamentals of Supported Catalysis I: Hydrocarbon Reactions
Thursday, Nov 2, 8:00 AM
MCC, L100F

Eleni A. Kyriakidou, Chair
Taejin Kim, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

8:00 Paper 661a: Methane Conversion to Ethylene and Aromatics on PtSn Catalysts — ***Duygu Gerceker***, *Ali Hussain Motagamwala, Keishla R. Rivera-Dones, James B. Miller, George W. Huber, Manos Mavrikakis, James A. Dumesic*

8:18 Paper 661b: Geometric and Electronic Effects of Zn Promotion on Pt for Ethane Dehydrogenation — *Viktor J. Cybulskis, Brandon C. Bukowski,* ***Han-Ting Tseng***, *James R. Gallagher, Zhenwei Wu, Evan C. Wegener, A. Jeremy Kropf, Bruce Ravel, Fabio H. Ribeiro, Jeffrey Greeley, Jeffrey T. Miller*

8:36 Paper 661c: CO, C_2H_2, and C_3H_6 Oxidation on Pd/Ceria-Zirconia/Al_2O_3 Three-Way Catalysts — ***Wendy Lang***, *Michael P. Harold, Yisun Cheng, Carolyn Hubbard, Paul Laing*

8:54 Paper 661d: Sintering and Deactivation Mechanism of Platinum/Palladium Two-Phase Catalysts — ***Luke T. Roling***, *Emmett Goodman, Matteo Cargnello, Frank Abild-Pedersen*

9:12 Paper 661e: Functional Descriptors, Active Intermediates, and the Influence of the Porous Environment for Epoxidations at Lewis Acidic Metal Atoms in Zeolite BEA — ***David W. Flaherty***, *Daniel T. Bregante*

9:30 Paper 661f: A Comparative Study of ZSM-5 and BEA Zeolites for Low-Temperature Passive Adsorption — ***Eleni A. Kyriakidou***, *Jae-Soon Choi, Todd J. Toops, James E. Parks*

9:48 Paper 661g: Kinetic Monte Carlo Simulation of Propylene Epoxidation on Supported Gold Nanoparticles — ***C. Heath Turner***, *Jingjing Ji, Zheng Lu, Yu Lei*

10:06 Paper 661h: A Computational Mechanism Study of Ethylene Dimerization and Hydrogenation on Iridium-Loaded Nu-1000 and UiO-66 — ***Hakan Demir***, *Christopher Cramer, Laura Gagliardi*

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(662) Going to a Decision Point in Sustainability Analysis
Thursday, Nov 2, 8:00 AM
MCC, 102E

Gonzalo Guillén-Gosálbez, Chair
Jose Maria Ponce-Ortega, Co-Chair

Sponsored by: Sustainability

8:00 Paper 662a: Bilevel Optimization Applied to the Exhaustive Exploration of Pareto Fronts in Sustainability Studies: Application to the Redesign of the UK Electricity Mix — ***Gonzalo Guillén-Gosálbez***, *Phantisa Limleamthong*

8:25 Paper 662b: Applying Emission Estimations, Pollution Controls, and Sustainability Evaluations for Generating Chemical Life-Cycle Inventories — ***Gerardo J. Ruiz-Mercado***, *Raymond L. Smith, Michael A. Gonzalez, David E. Meyer, Shuyun Li, Fernando V. Lima*

8:50 Paper 662c: A Decision Support Framework for Sustainable Manufacturing — ***Majid Moradi Aliabadi***, *Yinlun Huang*

9:15 Paper 662d: Techno-Ecological Synergies in Life-Cycle Assessment: A General Computational Framework — ***Xinyu Liu***, *Bhavik R. Bakshi*

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(663) Hydrothermal Carbonization
Thursday, Nov 2, 8:00 AM
MCC, 200E

Michael T. Timko, Chair
Catherine E. Brewer, Co-Chair

Sponsored by: Biorefinery Technologies for Forest-Based Lignocellulosic Biomass

8:00 Welcoming Remarks

8:10 Paper 663a: Design, Fabrication, Testing, and Operation of a Continuous Reactor for Hydrothermal Carbonization — ***Charles J. Coronella***, *Saeed Vahed Qaramaleki, M. Toufiq Reza*

8:30 Paper 663b: Fate of Nitrogen During Hydrothermal Treatment of Septage — ***Kyle McGaughy***, *Akbar Saba, M. Toufiq Reza*

8:50 Paper 663c: Hydrothermal Treatment of Paper Mill Sludge — ***M. Toufiq Reza***, *Kyle McGaughy*

9:10 Paper 663d: Structural Analysis of Humins Formed in the Brønsted-Catalyzed Dehydration of Fructose — ***Ziwei Cheng***, *Jeffrey Everhart, George Tsilomelekis, Vladimiros Nikolakis, Basudeb Saha, Dionisios G. Vlachos*

9:30 Paper 663e: Super-Oleophilic and Water-Repellent Graphene Oxide Sponge for Catalytic Coupling of Furanics — ***Saikat Dutta***, *Dionisios G. Vlachos, Basudeb Saha*

9:50 Paper 663f: Simultaneous Isomerization and Reactive Extraction Followed by Back Extraction of Sugars from Biomass Hydrolysate for High Purity and Yield of Ketose Sugars — ***Peng Zhang***, *Sasidhar Varanasi, Patricia Relue*

10:10 Concluding Remarks

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(664) Industrial Applications in Design and Operations
Thursday, Nov 2, 8:00 AM
MCC, 103E

Vijay Gupta, Chair
Zhihong Yuan, Co-Chair

Sponsored by:
Computers in Operations and Information Processing

8:00 Paper 664a: Maintenance Optimization-Based Survival Analysis for Optimal and Safer Operation: Cooling Tower Case Study — ***Prerna Jain***, *Efstratios N. Pistikopoulos, M. Sam Mannan*

8:19 Paper 664b: Scheduling and Feed Quality Optimization for Raw Materials in the Metals Industry — ***Yingkai Song***, *Brenno C. Menezes, Pablo Garcia-Herreros, Ignacio E. Grossmann*

8:38 Paper 664c: Overcoming a Lack of Data in Decision Analysis — ***Scott J. Bury***

8:57 Paper 664d: Mixed-Integer Nonlinear Programming Models for Line Pressure Optimization in Shale Gas Gathering Systems — *Markus G. Drouven,* ***Ignacio E. Grossmann***

9:16 Paper 664e: Optimal Startup of Hydrogen Plant Using Data-Driven Model — ***Abhinav Garg***, *Prashant Mhaskar, Ankur Kumar, Gangshi Hu, Jesus Flores-Cerrillo*

9:35 Paper 664f: Product-Centric Continuous-Time Formulation for Straight Pipelines — ***Pedro M. Castro***, *Hossein Mostafaei*

9:54 Paper 664g: An Optimization-Based Framework to Define the Probabilistic Design Space of Pharmaceutical Process with Model-Inherent Uncertainty — ***Shu Xu***, *Carl Laird, Salvador García-Muñoz, Shankar Vaidyaraman*

10:13 Paper 664h: Supply Chain Design of Continuous Tablet Manufacturing Facilities Using Discrete Event Simulation — ***Anne Purdy***, *Amy Greer, Palmerly Tom, Ondrej Slama, Pavlo Minayev, Vaclav Belak*

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(665) Innovations in Biopharmaceutical Discovery, Development, and Manufacturing
Thursday, Nov 2, 8:00 AM
MCC, 204A/B

Elcin Icten, Chair
Colin Walters, Co-Chair

Sponsored by:
Pharmaceutical Discovery, Development and Manufacturing Forum

8:00 Paper 665a: Impurity Rejection in Crystallization: Quantification and Mechanisms — ***Fredrik Nordstrom***

8:22 Paper 665b: Bi-Directional Control of Glycosylation of Antibodies — ***Madiha Khurshid***, *Tony Wang, Erin Franco, Nelson Chavez, Eleanor Le, Richard Wu, Randy Schweickart, J ack Chung-Jr Huang*

8:44 Paper 665c: Bioprocess Optimization for Production of Recombinant Proteins in Chinese Hamster Ovary Cells in Consideration of Metabolic Shifts by Shear Stress — ***Keisuke Shibuya***, *Kenichiro Oka*

9:06 Paper 665d: Using Machine Learning Tools in Bioprocess Scale-Up When the Number of Batches Is Small — ***Viktor Konakovsky***, *Graham McCreath, Jarka Glassey*

9:28 Paper 665e: A Workflow-Based Framework for Managing Product Analytical Data and Statistical Results for Lot Release — ***Girish Joglekar***, *Qing Cai, Poching DeLaurentis, Linas Mockus, Kenneth Morris, Gintaras V. Reklaitis*

9:50 Paper 665f: Evaluation of Recovery Pathways for Improved Bioavailability of Clofazimine Nanoparticles — ***Jie Feng***, *Yingyue Zhang, Hoang Lu, Simon A. McManus, Robert K. Prud'homme*

10:12 Paper 665g: Assessment of the Impact of Interfacial and Shear Stress on Biologics Drug Product via Mini-Piloting Tools — ***Maria Olu Ogunyankin***, *Smeet Deshmukh, Masano Huang, Thiago Carvalho, Mary Krause, Brenda Remy, Mehrnaz Khossravi*

(666) Integrated Product and Process Design
Thursday, Nov 2, 8:00 AM
MCC, 103C

Ravendra Singh, Chair
Kyle Camarda, Co-Chair

Sponsored by:
Systems and Process Design

8:00 Paper 666a: Assessment of Economic Potential of Furfural Platform — ***Sampath Gunukula***, *Hemant P. Pendse, William J. DeSisto, M. Clayton Wheeler*

8:21 Paper 666b: Economic and Modeling Analysis of Product- and Energy-Driven Biorefineries Based on Thermal Deoxygenation Pathway — ***Sampath Gunukula***, *Hemant P. Pendse, William J. DeSisto, Clayton Wheeler*

8:42 Paper 666c: An Algorithm for Integrated Design of Organic Rankine Cycles — *Uku Erik Tropp, David H. Bowskill, Smitha Gopinath, George Jackson, Amparo Galindo,* ***Claire S. Adjiman***

9:03 Paper 666d: Integrated Computational Design of Cosmetic Products — ***Cristhian D. Tinjacá***, *Juan J. Torres, Jorge M. Gómez, Oscar Alvarez*

9:24 Paper 666e: Modeling and Multi-Objective Optimization of an Industrial Ammonia Synthesis Process — *Stanislav Ivanov,* ***Ajay K. Ray***

9:45 Paper 666f: Generation of Sustainable Hybrid Process Flowsheets Using PROCAFD — ***Anjan Kumar Tula***, *Mario Richard Eden, Rafiqul Gani*

10:06 Paper 666g: Total Site Integration as a Synthesis Tool to Select Biomass Valorization Paths and Schedule Multiple-Feedstock Operations — ***Konstantinos A. Pyrgakis***, *Antonis C. Kokossis*

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(667) Integrated Production Scheduling and Control
Thursday, Nov 2, 8:00 AM
MCC, 103D

Donald J. Chmielewski, Chair
Debangsu Bhattacharyya, Co-Chair

Sponsored by:
Systems and Process Control

8:00 Paper 667a: Grid-Level "Battery" Operation of Chemical Processes with Engagement in Short-Term Electricity Markets — ***Joannah Otashu***, *Michael Baldea*

8:17 Paper 667b: A Decomposition Approach for the Integration of Scheduling and Model Predictive Control in Fast-Changing Market Conditions — ***Lisia S. Dias***, *Richard Pattison, Michael Baldea, Marianthi Ierapetritou*

8:34 Paper 667c: On the Design of an Online Scheduling Algorithm — ***Dhruv Gupta***, *Christos T. Maravelias*

8:51 Paper 667d: Unified Treatment of Scheduling and Control: Same Story, Different Dynamics? — ***Michael Risbeck***, *Christos T. Maravelias, James B. Rawlings*

9:08 Paper 667e: Dynamic Scheduling to Maximize the Profitability of Air Separation Units — ***Song Wang***, *Qiang Xu, Jian Zhang, Zhenlei Wang*

9:25 Paper 667f: Investigation of Closed-Loop Optimal Process Scheduling Policies — ***Yazeed Aleissa***, *Donald J. Chmielewski*

9:42 Paper 667g: Integration of Design, Scheduling and Control Under Uncertainty via Model-Based Multi-Parametric Programming — ***Baris Burnak***, *Justin Katz, Nikolaos A. Diangelakis, Efstratios N. Pistikopoulos*

9:59 Paper 667h: Superstructure-Based Process Synthesis of a Pre-Combustion Membrane CO_2 Capture System — ***Michael Matuszewski***, *Lorenz T. Biegler*

10:16 Paper 667i: Data-Driven Modelling and Optimization for Managing the Load Distribution of Electric Motor-Operated Compressors — ***Hamza Hamadah***, *Nina F. Thornhill, Dionysios Xenos*

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(668) Integrated Thermochemical and Biochemical Processing for Renewable Fuels and Chemicals
Thursday, Nov 2, 8:00 AM
MCC, 101D

Christopher M. Saffron, Chair
Hema Ramsurn, Co-Chair

Sponsored by:
Sustainable Biorefineries

8:00 Paper 668a: Development CO Sensor for Syngas Fermentation for Production of Fuels and Chemicals — *Jie Dang, Ning Wang,* ***Hasan K. Atiyeh***

8:25 Paper 668b: Techno-Economic Analysis (TEA) of a Novel Hybrid Enzyme- and Chemo-Catalytic Process for Producing Furans from Biomass Hydrolysate — ***Ravikumar Gogar***, *Sridhar Viamajala, Patricia Relue, Sasidhar Varanasi*

8:50 Paper 668c: Electrocatalytic Hydrogenation of Lignin-Derived Bio-Oil Model Compounds Using Ruthenium on Activated Carbon Cloth to Produce Liquid Fuel Intermediates and Value-Added Products — ***Mahlet Garedew***, *Daniel Frahat-Young, James E. Jackson, Christopher M. Saffron*

9:15 Paper 668d: Thermal Deconstruction Opens Biomass for Acid Hydrolysis to Sugars — ***Jake K. Lindstrom***, *Peter N. Ciesielski, Chad Peterson, Juan Proano-Aviles, Preston A. Gable, Robert C. Brown*

9:40 Paper 668e: Fermentable Sugar Production from Biomass Using THF/Water and Dilute Acid Catalyst — ***Arpa Ghosh***, *Robert C. Brown*

10:05 Paper 668f: Optimization and Performance Improvement of Bioethanol Biorefinery Through the Integration of Thermochemical-Utilized Lignin Residue — ***Nasir Al Lagtah***

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(669) Interfacial Aspects of Oil/Gas Recovery and Remediation
Thursday, Nov 2, 8:00 AM
MCC, M100B

James W. Schneider, Chair
Marina Tsianou, Co-Chair
Clint P. Aichele, Co-Chair

Sponsored by:
Interfacial Phenomena

8:00 Paper 669a: Impact of Molecular Structure on Surface and Thermal Properties of Amido-Amine Cationic Gemini Surfactants — ***Muhammad Shahzad Kamal***, *S. M. Shakil Hussain, Abdullah S. Sultan*

8:15 Paper 669b: Surfactant Effect on Hydrate Crystallization at Oil-Water Interface — ***Liat Rosenfeld***, *Kevin Dann*

8:30 Paper 669c: Surface Tension Behavior of Aqueous Solutions of a Propoxylated Surfactant and Interfacial Tension Behavior Against an Un-Preequilibrated Crude Oil — ***Jaeyub Chung***, *Bryan W. Boudouris, Elias I. Franses*

8:45 Paper 669d: Eco-Friendly Sacrificial Amphiphiles as Chemical Herders for Oil Spill Remediation — ***Hao Zhou***, *George John, Charles Maldarelli*

9:00 Paper 669e: Interfacial Interactions in Oil/Brine Emulsions Stabilized by Combinations of Cellulose Nanocrystals and Emulsion Stabilizers — ***Sanjiv Parajuli***, *Chadwick E. Middleton, Andres E. Rodriguez Zambrano, Esteban E. Ureña-Benavides*

9:15 Paper 669f: Measurement and Surface Complexation Modeling of Calcite Zeta Potential in Mixed Brines for Carbonate Wettability Characterization — ***Jin Song***, *Yongchao Zeng, Xindi Duan, Le Wang, Walter Chapman, Sibani L. Biswal, George J. Hirasaki*

9:30 Paper 669g: Dissolution and Restructuring of Calcite Surfaces in Contact with Electrolyte Solutions: Implications for Enhanced Oil Recovery — ***Kai Kristiansen***, *Szu-Ying Chen, Yair Kaufman, Nicholas Cadirov, Howard Dobbs, Alex Schrader, Dongjin Seo, J. Boles, J. N. Israelachvili*

9:45 Paper 669h: Marine Bacteria Adhesion to Oil/Water Interfaces — *Michael Godfrin, Maswazi Sihlabela,* ***Arijit Bose***, *Anubhav Tripathi*

10:00 Paper 669i: Oil Spill Dispersion with Food-Grade Amphiphiles: Formation of Oil-Bacteria Agglomerates During Oil Biodegradation — ***Geoffrey D. Bothun***, *Joseph Rocchio, Srinivasa R. Raghavan, Vijay T. John, Alon McCormick*

10:15 Paper 669j: The Role of Bacterial Biofilm in Particle-Stabilized Oil-in-Water Emulsions: Implications to the Biodegradation of Oil Spills — ***Marzhana Omarova***, *Lauren T. Swientoniewski, Diane A. Blake, Geoffrey D. Bothun, Vijay T. John*

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(670) Lithium and Beyond: Fundamental Advances in High-Performance Batteries I
Thursday, Nov 2, 8:00 AM
MCC, M100C

Paul Kohl, Chair
John Staser, Co-Chair
Nian Liu, Co-Chair

Sponsored by:
Electrochemical Fundamentals

8:00 Paper 670a: Novel Cathode Materials for Rechargeable Aluminum Batteries — ***Robert J. Messinger***, *Jeffrey Xu, Ankur Jadhav*

8:20 Paper 670b: Reversibility of Zinc Metal Anode: Fundamentals and Engineering — ***Nian Liu***

8:40 Paper 670c: An Air-Breathing Lithium-Oxygen Battery — ***Baharak Sayahpour***, *Mohammad Asadi, Pedram Abbasi, Larry A. Curtiss, Amin Salehi-Khojin*

9:00 Paper 670d: Appropriate Characterization Techniques for Lithium-Oxygen Batteries, and Implications for Understanding 2e- vs. 4e- Oxygen Reduction Processes — ***Colin M. Burke***, *Bryan D. McCloskey*

9:20 Break

9:30 Paper 670e: Mechanistic Insights into the Sodium-Oxygen Battery Cathode Electrochemistry
— ***Jessica E. Nichols***, *Bryan D. McCloskey*

9:50 Paper 670f: Mechanistic Evaluation of Thermal Runaway in Potassium-Ion Batteries
— ***Ryan A. Adams***, *Arvind Varma, Vilas G. Pol*

10:10 Paper 670g: Molten Salt Batteries: Mechanics and Electrolyte Transport — ***Christine Cardinal Roberts***, *Martin B. Nemer, Mark Stavig, Alexander Headley, Ryan Solich, Scott A. Roberts*

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(671) Materials Science in Pharmaceutical Process Development I
Thursday, Nov 2, 8:00 AM
MCC, 205D

Jason Mustakis, Chair
Lei Zhu, Co-Chair

Sponsored by:
Pharmaceutical Discovery, Development and Manufacturing Forum

8:00 Paper 671a: Suitable Raw Material Attributes for Continuous Manufacturing of a Drug Product via Direct Compression — ***Brendon G. Ricart***

8:20 Paper 671b: Material Sparing Approach to Predict API Performance in Direct Compaction — ***Pallavi Pawar***, *Abdenour Djemai*

8:40 Paper 671c: Wettability of Pharmaceutical Powders of Different Particle Size by Droplet Penetration Technique — *Yu Han, Zhanjie Liu,* ***Sara Moghtadernejad***, *Fernando Muzzio, Gerardo Callegari, German Drazer*

9:00 Paper 671d: Investigation of Microsphere Strength for Spray-Drying Applications by Means of Acoustic Levitation — ***Manuel Kreimer***, *Isabella Aigner, Stephan Sacher, Markus Krumme, Thomas Mannschott, Peter van der Wel, Albert Kaptein, Hartmuth Schröttner, Günter Brenn, Johannes G. Khinast*

9:20 Paper 671e: Nanostructural Interfaces of Additives on the API Surfaces Influencing Process Performance — ***Sajan K. Chatarla***, *Tijana Rajh, Elena Rozhkova, Kalyana Pingali*

9:40 Paper 671f: Rational Strategies for Physical Characterization of Amorphous Solid Dispersions During Drug Product Development and Manufacture — ***Stephen L. Conway***, *Kenneth Rosenberg, Itzia Arroyo, Andrew Gmitter, Julianne Farabaugh, Cindy Starbuck*

10:00 Paper 671g: Investigation of Compression-Induced Amorphization of Crystalline API — ***Lei Zhu***, *Chengbin Huang, Gerard Klinzing, Adam Procopio, Fengyuan Yang, Jie Ren, Rubi Burlage, Anthony Leone, Lawrence Rosen, Yongchao Su*

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(672) Membranes for CO_2 Separations — GS IV
Thursday, Nov 2, 8:00 AM
MCC, M100I

Dhaval Bhandari, Co-Chair
Surinder Singh, Co-Chair
Michele Galizia, Co-Chair

Sponsored by:
Membrane-Based Separations

8:00 Paper 672a: CO_2-Philic Polymer Membranes for High-Flux CO_2 Separation — *Tao Hong, Pengfei Cao, Bingrui Li, Hongbo Feng, Shannon Mahurin, De-en Jiang, Konstantinos Vogiatzis, Jimmy W. Mays, Brian Long, Alexei Sokolov,* ***Tomonori Saito***

8:18 Paper 672b: Highly Cross-Linked Polymers for Membrane H_2/CO_2 Separation at Elevated Temperatures — ***Maryam Omidvar***, *Mark T. Swihart, Haiqing Lin*

8:36 Paper 672c: High-Throughput Direct Synthesis of CuBDC MOF Nanosheets and Their Application in CO_2 Separation — ***Meera Shete***, *Jonathan E. Bachman, Zachary P. Smith, Xiaoli Ma, Jeffrey R. Long, Michael Tsapatsis*

8:54 Paper 672d: New Negative Emissions Technology: Indirect Ocean Capture Separating CO_2 from Air — ***Charles-François de Lannoy***, *Matthew Eisaman, Jessy Rivest, Stephen Karnitz, Arun Jose, Richard DeVaul, Kathy Cooper*

9:12 Paper 672e: Study of Carrier Saturation Phenomenon in Facilitated Transport Membrane for CO_2 Capture from Low–CO_2 Concentration Sources — ***Dongzhu Wu***, *Yang Han, W. S. Winston Ho*

9:30 Paper 672f: High-Performance Hydroxyl-Functionalized Polyimides for Natural Gas Separation — ***Nasser Alaslai***, *Bader Ghanem, Fahd I. Alghunaimi, Ingo Pinnau*

9:48 Paper 672g: Recent Applications of Separex Membranes Beyond CO_2 Removal — ***Simon E. Albo***, *Alex Cedillo, Steve Poklop, Ganesh Nayak, Lixiao Zeng, Clemence Peng, Qing Xu, Lisa Wolschlag*

10:06 Paper 672h: A New Experimental Technique for the Study of Gas Permeation of Binary Mixture — ***Kean Wang***, *Zhou He*

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(673) Mixing and Segregation of Particulate Systems I
Thursday, Nov 2, 8:00 AM
MCC, 200J

Richard M. Lueptow, Chair
Ben Freireich, Co-Chair

Sponsored by:
Solids Flow, Handling and Processing

8:00 Paper 673a: Changing the Mass Flow Limit: What Bin Designs Will Minimize Segregation and How Do We Change the Mass Flow Limit to Optimize Segregation Prevention? — ***Kerry Johanson***

8:18 Paper 673b: Multilayer Granular Segregation in Discharging Cylindrical Hoppers — ***Manogna Adepu***

8:36 Paper 673c: DEM Investigation of Adhesive Mixing of Fine and Coarse Particles: Dynamics of Collisional Mixing and Attachment — *Xiaoliang Deng, Kai Zheng,* ***Rajesh N. Dave***

8:54 Paper 673d: Improved Pharmaceutical Blend Content Uniformity Due to Reduced Agglomeration of Dry-Coated Micronized Drug Powders — *Zhonghui Huang, Kuriakose Kunnath,* ***Rajesh N. Dave***

9:12 Paper 673e: Segregation of Fragile Granular Materials — ***Ben Freireich***, ***Yi Fan***, *Karl Jacob*

9:30 Paper 673f: Lubrication in Continuous Tubular Powder Blenders — *Sarang Oka,* ***Sara Moghtadernejad***, *Zhanjie Liu, Fernando J. Muzzio*

9:48 Paper 673g: Particle Size Segregation in Granular Shear Flows — ***Siying Liu***, *J. J. McCarthy*

10:06 Paper 673h: Quantification of Granular Size Segregation in a 3D Conical Bounded Heap: Theory, Simulations, and Experiments — *Austin B. Isner, Paul B. Umbanhowar, Julio M. Ottino,* ***Richard M. Lueptow***

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(674) Modeling and Engineering Cellular Communities
Thursday, Nov 2, 8:00 AM
MCC, 208A

Rajib Saha, Chair
Ophelia S. Venturelli, Co-Chair

Sponsored by: Bioengineering

8:00 Paper 674a: SteadyCom: Modeling Microbial Communities Under Steady-State Growth — ***Siu Hung Joshua Chan***, *Margaret Simons-Senftle, Costas D. Maranas*

8:18 Paper 674b: Intracellular Metabolic Circuits Shape Intercellular Interactions in Multi-Species Microbial Games — ***Ali R. Zomorrodi,*** *Daniel Segrè*

8:36 Paper 674c: Elucidating Parameters in Dynamic Microbial Community Models Using Nonlinear Programming — ***Sungho Shin***, *Ophelia S. Venturelli, Victor M. Zavala*

8:54 Paper 674d: Constraint-Based Community Modeling Reveals Condition-Dependent Alternate Interactions — ***Cristal Zuniga P***, *Karsten Zengler*

9:12 Paper 674e: Engineered Biofilms for Isobutanol Production: In-Silico Modeling of a Two-Species Bacterial Community — ***Michael A. Henson***, *Ayushi Patel, Ross P. Carlson*

9:30 Paper 674f: Microbiome-Virome Interactions in Bovine Rumen: The Role of Auxiliary Metabolic Genes in Relaxing Metabolic Bottlenecks — ***Mohammad Mazharul Islam***, *Wheaton Schroeder, Rajib Saha, Samodha C. Fernando*

9:48 Paper 674g: Development and Application of Integrated Pipeline for the Modeling and Analysis of Microbial Communities in the DOE Systems Biology Knowledgebase — ***Christopher S. Henry,*** *Pamela Weisenhorn, José P. Faria, Janaka N. Edirisinghe, Ronald C. Taylor, Hyun-Seob Song, Hans C. Bernstein, Jeremy Zucker, Stephen R. Lindemann, Adam P. Arkin*

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(675) Molecular Modeling of Industrially Relevant Interfacial Phenomena
Thursday, Nov 2, 8:00 AM
MCC, L100H

Jindal K. Shah, Chair
Martin Sanborn, Co-Chair

Sponsored by:
Computational Molecular Science and Engineering Forum

8:00 Paper 675a: Uncovering Heterogeneous Ice Nucleation Using Advanced Molecular Simulations [Invited Talk] — ***Sapna Sarupria***, *Brittany Glatz*

8:30 Paper 675b: Investigation of the Chromatographic Separation of Chiral Drugs by Molecular Dynamics Simulation — ***Binwu Zhao***, *David W. House, Xiaoyu Wang, Priyanka Oroskar, Anil Oroskar, Asha Oroskar, Cynthia J. Jameson, Sohail Murad*

8:45 Paper 675c: Molecular Simulation of CO_2 Absorption in Sorbent-Solvent Suspension and Interface Regions — ***Wei Shi***, *David Hopkinson*

9:00 Paper 675d: Acid Gas Adsorption on Metal–Organic Framework Nanosheets as a Model of an "All-Surface" Material — ***Joshua Howe***, *Yang Liu, Luis Flores, David A. Dixon, David S. Sholl*

9:15 Paper 675e: Contaminant Adsorption on α-Alumina Surface as Predicted by the Plane-Wave Density Functional Theory — ***Manoj Shukla***

9:30 Paper 675f: Conformal Sites Model for Adsorbed Films on Energetically Heterogeneous Surface — ***Kaihang Shi***, *Erik E. Santiso, Keith E. Gubbins*

9:45 Paper 675g: Identifying Relationships Between Terminal Group Chemistry and Interfacial Friction in Monolayer-Based Lubrication Through a Molecular Dynamics Screening Approach — ***Andrew Z. Summers***, *Christopher R. Iacovella, Peter T. Cummings, Clare McCabe*

10:00 Paper 675h: Molecular Simulation Study of Aluminum–Noble Gas Interfacial Thermal Accommodation Coefficients — ***Haoyan Sha***, *Roland Faller*

10:15 Paper 675i: The Water Flow Through Graphene Slit Pores: Insights from Non-Equilibrium Molecular Dynamics Simulations — ***Mingjie Wei***, *Fang Xu, Yong Wang*

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(676) Nanoscale Science and Engineering in Biomolecular Catalysis I
Thursday, Nov 2, 8:00 AM
MCC, 212A/B

Su Ha, Chair
Jungbae Kim, Co-Chair
Ping Wang, Co-Chair

Sponsored by: Bionanotechnology

8:00 Paper 676a: Targeted Killing of Pathogenic Bacteria with Cell Wall Binding Domain (CBD)-Antimicrobial Nanoparticle Conjugates — *Domyoung Kim, Seok-Joon Kwon, Inseon Lee, Jahyun Nam, Jungbae Kim,* ***Jonathan S. Dordick***

8:30 Paper 676b: Magnetic Polydopamine Nanotubes for Enhanced Enzyme Activity and Stability — *Chao Chen, Xiaoli Wang, Yibing Wang,* ***Ping Wang***

9:00 Break

9:10 Paper 676c: Magnetic Carbonic Anhydrase Nanogel for Enhanced CO_2 Sequestration — ***Weina Xu***, *Zheyu Wang, Gong Chen, Zhongwang Fu, Zheng Liu*

9:30 Paper 676d: Fabricating Multi-Enzyme Catalyst in Reverse Emulsions — ***Zheyu Wang***, *Weina Xu, Zhongwang Fu, Guoqiang Jiang, Zheng Liu*

9:50 Paper 676e: Tuning Electrochemical Performances of Glucose Oxidase Nanocomposites by Changing the Shape and Surface Properties of Carbon Support Materials — ***Tsai Garcia-Perez***, *Jungbae Kim, Su Ha*

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(677) NH_3 Fuel Synthesis I
Thursday, Nov 2, 8:00 AM
MCC, 101F/G

Sponsored by:
NH_3 Energy$^+$ — Enabling Optimized, Sustainable Energy and Agriculture

8:00 Paper 677a: Atmospheric-Pressure Synthesis of Ammonia Using Non-Thermal Plasma with the Assistance of Ru-Based Multifunctional Catalyst — ***Peng Peng***, *Yanling Cheng, Nan Zhou, Raymond Hatzenbeller, Paul Chen, Roger Ruan*

8:18 Paper 677b: Coupling Integral Molten Salt Reactor Technology into Hybrid Nuclear: Direct Ammonia Production via H_2 High-Temperature Steam Electrolysis — ***John Kutsch***

8:36 Paper 677c: Design of Iron-Nickel Nanocatalysts for Low-Temperature Electrochemical Ammonia Generation — *Shelby Foster, Prashant Acharya, David Suttmiller, Charles Loney, Julie N. Renner, Wayne Gellett, Katherine Ayers,* ***Lauren F. Greenlee***

8:54 Paper 677d: Early Transition Metal Carbide- and Nitride-Supported Catalysts for Ammonia Synthesis — ***Zixuan Wang***, *Levi T. Thompson*

9:12 Paper 677e: High-Efficiency Electrochemical Synthesis of Ammonia from Nitrogen at Ambient Temperature and Pressure — ***Greg Redden***, *Fengling Zhou, Luis Azofra, Muataz Ali, Mega Kar, Alexandr Simonov, Ciaran McDonnell, Chenghua Sun, Angeline Bartholomeusz, Xinyi Zhang, Douglas MacFarlane*

9:30 Paper 677f: Influence of H_2/N_2 Ratio on Dynamic Behavior of Ammonia Production on Ru Catalyst Under Low Pressure Condition — ***Hideyuki Matsumoto***, *Javaid Rahat, Tetsuya Nanba*

9:48 Paper 677g: LiH-Mediated Ammonia Synthesis Under Mild Condition — *Jianping Guo,* ***Ping Chen***

10:06 Paper 677h: Load Range Enhancement of Haber-Bosch Process Designs for NH_3 Sustainable Energy Storage by Multi-Parametric Optimization — ***Izzat Iqbal Cheema***, *Florian Baakes, Ulrike Krewer*

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(678) Novel Materials and Processes for Air Pollution Control
Thursday, Nov 2, 8:00 AM
MCC, 103B

Steven Ogunwumi, Chair
Bin Mu, Co-Chair
Yunfa Chen, Co-Chair

Sponsored by:
Innovations of Green Process Engineering for Sustainable Energy and Environment

8:00 Paper 678a: Propane Adsorption on ZIF-8 — ***Brice A. Russell***, *Aldo Migone*

8:18 Paper 678b: Conformal Zr-Based Metal-Organic Framework Thin Films on Nanofibers for Ultra-Fast Degradation of Chemical Warfare Agents — ***Junjie Zhao***, *Dennis T. Lee, Heather F. Barton, Robert W. Yaga, Morgan G. Hall, Ian R. Woodward, Christopher J. Oldham, Howard J. Walls, Gregory W. Peterson, Gregory N. Parsons*

8:36 Paper 678c: Engineering Copper Carboxylate Functionalities on Water-Stable Metal-Organic Frameworks for Enhancement of Ammonia Removal Capacities — ***Jayraj Joshi***

8:54 Paper 678d: A Combined Molecular Simulation and Process Simulation Study of Benzene Removal from Vinyl Acetate in MOFs — *Zhongdong Gan, Xiuqin Dong, Yifei Chen, Haoxi Jiang,* ***Minhua Zhang***

9:12 Paper 678e: New Strategies of Enhancing Steam Stability of MOFs by Modification with Post-Synthesis and In-Situ Synthesis Methods — ***Jing Xiao***, *Zhedong Lin, Hao Li, Xin Zhou, Zhong Li*

9:30 Paper 678f: High-Performance Gas Adsorption and Separation of Light Hydrocarbon in a Microporous Metal-Organic Framework — ***Feng Xu***, *Xin Chen*

9:48 Paper 678g: Emission of Sulphur- and Nitrogen-Based Pollutants in Commercial-Scale Circulating Fluidized Bed Gasifiers — ***Zhen Chai***, *ZhiPing Zhu, KuangShi Yu, Weiwei Liu, Haixiang Zhang*

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(679) Novel Nanoparticles and Nanostructured Materials for Energy & Environmental Applications I
Thursday, Nov 2, 8:00 AM
MCC, 200H

Yangchuan Xing, Chair
Satish Nune, Co-Chair
Alan W. Weimer, Co-Chair

Sponsored by: Nanoparticles

8:00 Paper 679a: Reactive Precipitation of Anhydrous Alkali-Sulfide Nanocrystals with Concomitant Abatement of Hydrogen Sulfide and Co-Generation of Hydrogen (Invited) — ***Colin A. Wolden***, *Xuemin Li, Yongan Yang, Yangzhi Zhao*

8:40 Paper 679b: Tunable Magnetic Core-Shell Nanoparticles: An Interplay Between Composition, Size, Shape and Architecture — *Natalia da Silva Moura, Hunter Simonson, Claire Boudreaux, Jacob Bursavich, Roshan Nepal, Rongying Jin, Zhen Wang,* ***James Dorman***

9:00 Paper 679c: Effects of Alumina Incorporation by Particle Atomic Layer Deposition on Sintering, Microstructure, and Ionic Conductivity of Yttria-Stabilized Zirconia (8YSZ) — ***Christopher J. Bartel***, *Rebecca O'Toole, Maila Kodas, Sandrine Ricote, Neal P. Sullivan, Austin Drake, Alexa Horrell, Robert Hall, Charles B. Musgrave, Alan W. Weimer*

9:20 Paper 679d: Atomic Layer Deposition Surface-Functionalized Adsorbents for Adsorption of Metal Ions and Organic Pollutants — ***Xiaofeng Wang***, *Xinhua Liang*

9:40 Paper 679e: Atomic Layer Deposition for Extended Surface Electrocatalyst Development — ***William McNeary IV***, *Katherine Hurst, Shaun M. Alia, Scott A. Mauger, K. C. Neyerlin, Chilan Ngo, J. W. Medlin, Alan W. Weimer, Svitlana Pylypenko, Karen J. Buechler, Bryan S. Pivovar*

10:00 Paper 679f: Ultrathin Hollow Graphene Oxide Membranes for Use as Nanoparticle Carriers for Energy and Biomedical Applications — ***Kurt B. Smith***, *M. Silvina Tomassone*

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(680) Polymer Thin Films and Interfaces
Thursday, Nov 2, 8:00 AM
MCC, 211C

Stephen M. Martin, Chair
Keith M. Forward, Co-Chair

Sponsored by: Polymers

8:00 Paper 680a: Molecular Simulations of the Influence of Interfaces on the Dynamics of Polymers — ***Robert A. Riggleman***

An up-to-date program is available at www.aiche.org/annual or on the Annual Meeting app
Please refrain from photographing slides or taking video of sessions and presentations.

TECHNICAL SESSIONS 2017

8:30 Paper 680b: Princess and the Pea Behavior in Polyelectrolyte Multilayers: Influence of the First Layer on Polyelectrolyte Multilayer Assembly and Properties — *Xuejian Lyu, **Amy M. Peterson***

8:45 Paper 680c: Instability of Liquid Crystal Thin Film on Topographically Patterned Substrates — ***Palash Dhara**, Rabibrata Mukherjee*

9:00 Paper 680d: Electroless Deposition of Copper on Quaternized Chitosan Coatings for Antibacterial Application — ***Debirupa Mitra**, En-Tang Kang, Ramanathan Kollengode, Matthew Cove, Koon Gee Neoh*

9:15 Paper 680e: Patterning Buckles in Polymer/Metal Thin Films by Laser Irradiation — ***Kunal Mondal**, Ying Liu, Michael D. Dickey, Jan Genzer*

9:30 Paper 680f: High-Performance Conducting Polymer Coatings for Corrosion Protection — ***Xinyu Zhang**, Amit Nautiyal, Jonathan Cook*

9:45 Paper 680g: Enhanced Wetting Stability of Initiated Chemical Vapor Deposited (iCVD) Polydivinylbenzene Thin Films by Thermal Annealing — ***Junjie Zhao**, Minghui Wang, Karen K. Gleason*

10:00 Paper 680h: Nanoscale Characterization of Water Penetration Through Plasma Polymerized Coatings and Water at the Coating/Substrate Interface — *Yang Zhou, Ali Dhinojwala, **Mark Foster***

10:15 Paper 680i: Surface Topology and Modulus Effects on Adhesion in Novel Polyorganosiloxane-Based Coatings — ***Ethan D. Smith**, Stephen M. Martin, Vince Baranauskas*

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(681) Process Design: Innovation for Sustainability
Thursday, Nov 2, 8:00 AM
MCC, 101C

Gerardo J. Ruiz-Mercado, Chair
Heriberto Cabezas, Co-Chair
Yuan Yao, Co-Chair

Sponsored by: General

8:00 Paper 681a: Screening for Economically Promising Bio-Based Chemicals — ***Wenzhao (Tony) Wu**, Matthew Long, Jennifer Reed, Christos T. Maravelias*

8:25 Paper 681b: Supercritical Fluid Carnot Cycle for Low-Temperature Waste Heat Utilization — ***Madeleine Laitz**, Eldred Chimowitz, Doug Kelley*

8:50 Paper 681c: Designing Techno-Ecological Synergies While Accounting for Ecosystem Dynamics — *Varsha Gopalakrishnan, **Bhavik R. Bakshi***

9:15 Paper 681d: Design and Dynamic Simulation of a Solar and Natural Gas Hybrid Power Plant to Investigate the Synergies of Hybridization — ***Khalid Rashid**, Kody M. Powell*

9:40 Paper 681e: The Design of Sustainable Carbon Dioxide Capture and Conversion Processes Considering Various Locations, Products and Routes — ***Rebecca Frauzem**, John M. Woodley, Rafiqul Gani*

10:05 Paper 681f: Optimal Integrated Plant for Waste-to-Biodiesel Production — *Borja Hernández, **Mariano Martin***

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(682) Molecular Simulation of Adsorption II
Thursday, Nov 2, 8:00 AM
MCC, M100E

Peter I. Ravikovitch, Chair
Li-Chiang Lin, Co-Chair

Sponsored by: Adsorption and Ion Exchange

8:00 Paper 682a: Insights and Rational Design of Metal-Organic Frameworks for Enantiomers Separations — ***Tim Duerinck**, Joeri Denayer, Randall Q. Snurr*

8:17 Paper 682b: Selective Carbohydrate Adsorption in Solvated Nu-1000 — ***Hakan Demir**, Christopher Cramer, Laura Gagliardi*

8:34 Paper 682c: Molecular Simulation of Combined Chemi- and Physi-Sorption of Carbon Monoxide on Cobalt in the Presence of Supercritical Hexane — *Carrie Veer, Christer Karlsson, **Kenneth M. Benjamin***

8:51 Paper 682d: Atomistic Understandings of the CO_2 Uptake Difference in Photo-Responsive Metal-Organic Frameworks — ***Chi-Ta Yang**, Azzam Charaf Eddin, Roberta Poloni, Li-Chiang Lin*

9:08 Paper 682e: Sorption-Relaxation Behavior in Polymers of Intrinsic Microporosity During Gas Separation from Molecular Simulations — ***Grit Kupgan**, Michael E. Fortunato, Alexander Demidov, Coray M. Colina*

9:25 Paper 682f: Framework Flexibility–Driven Adsorptive Separation of C_8 Aromatic Isomers in Metal-Organic Frameworks: A Computational Exploration — ***Mayank Agrawal**, David Sholl*

9:42 Paper 682g: Molecular Simulation Studies Probing Transport and Adsorption of C_8 Aromatics Through MFI Nanosheet Membranes — ***Raghuram Thyagarajan**, Evgenii Fetisov, Robert F. DeJaco, Peng Bai, Michael Tsapatsis, J. Ilja Siepmann*

9:59 Paper 682h: Computational Screening of Zeolites for Gas Separation Applications from Multi-Component Mixtures — ***Shachit S. Iyer**, Salih E. Demirel, M. M. Faruque Hasan*

10:16 Paper 682i: Unraveling of Pristine and Defective Metal-Organic Framework (MOF) Structures Through Molecular Simulation — *Ryther Anderson, Cornelius Audu, Peng Li, Omar K. Farha, SonBinh Nguyen, **Diego Gomez Gualdron***

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(683) Nucleation and Growth
Thursday, Nov 2, 8:00 AM
MCC, M100J

Venkateswarlu Bhamidi, Chair
Ryan C. Snyder, Co-Chair

Sponsored by: Crystallization and Evaporation

8:00 Welcoming Remarks

8:05 Paper 683a: Entropy-Driven, Two-Step Crystallization of Colloidal Clathrate Crystal — ***Sangmin Lee**, Michael Engel, Sharon C. Glotzer*

8:25 Paper 683b: Unraveling the Coupling Between Demixing and Crystallization in Mixtures — ***Jerome Delhommelle**, Caroline Desgranges*

8:45 Paper 683c: La Mer Burst Nucleation and Growth: Assumptions, Models, and Data — ***Baron Peters***

9:05 Paper 683d: A Stochastic Model of Primary Nucleation of Polymorphs — ***Giovanni Maria Maggioni**, Leonard Bezinge, Marco Mazzotti*

9:25 Paper 683e: Step Velocity of a Crystal Edge with Alternating Rows of Growth Units — ***Mark Joswiak**, Baron Peters, Michael F. Doherty*

9:45 Paper 683f: Multiscale, Multiphysics, Mechanistic Model for Computation of Face-Specific Growth Rates — ***James Fell**, Anish V. Dighe, Meenesh R. Singh*

10:05 Paper 683g: Anisotropic Growth Kinetics of Triblock Janus Colloids — ***Wesley F. Reinhart**, Athanassios Z. Panagiotopoulos*

10:25 Concluding Remarks

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(684) Rational Catalyst Design I: Computational Approach
Thursday, Nov 2, 8:00 AM
MCC, L100A

Zhenmeng Peng, Chair
Adam Holewinski, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

8:00 Paper 684a: A Simple Coordination-Based Model for Bimetallic Nanoparticles — ***Luke T. Roling**, Frank Abild-Pedersen*

8:20 Paper 684b: Design of Metallic Surface Nanostructures Using Mathematical Optimization — ***Christopher L. Hanselman**, Chrysanthos E. Gounaris*

8:40 Paper 684c: Accelerated Catalyst Screening Using Computational Alchemy — ***Karthikeyan Saravanan**, John R. Kitchin, O. Anatole von Lilienfeld, John A. Keith*

9:00 Paper 684d: DFT Study of Trends in Reactivity at Bifunctional Interfaces: A Case Study of Water-Gas Shift on Doped Au/MgO — ***Paulami Majumdar**, Tej S. Choksi, Jeffrey P. Greeley*

9:20 Paper 684e: Perovskite Oxides for Low-Temperature Carbon Dioxide Conversion Towards Hydrocarbon Generation — ***Debtanu Maiti**, Bryan J. Hare, Yolanda Daza, Adela E. Ramos, John Kuhn, Venkat R. Bhethanabotla*

9:40 Paper 684f: Design of Ruddlesden-Popper Oxides with Optimal Activity for Surface Oxygen Exchange and Electrochemical Oxygen Reduction — ***Nuwandi M. Ariyasingha**, Xiang-Kui Gu, Juliana S. A. Carneiro, Anirban Das, Eranda Nikolla*

10:00 Paper 684g: Identification of Highly Active Catalytic Sites for Oxygen Reduction Reaction in Carbon Nanostructures from First-Principles Investigation — ***Gregory Hartmann**, Gyeong Hwang*

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(685) Recent Advances in Molecular Simulation III: Free Energy and Phase Equilibrium
Thursday, Nov 2, 8:00 AM
MCC, L100J

Francisco R. Hung, Chair
Erik E. Santiso, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

8:00 Paper 685a: Enhanced Sampling Methods for Modulating Density Fields — *Zhitong Jiang, Suruchi Fialoke, **Amish Patel***

8:19 Paper 685b: Mapped Averaging Methods for Accurate and Precise Evaluation of Free Energies and Other Properties by Molecular Simulation — *Weisong Lin, Akshara Goyal, Sabry G. Moustafa, Andrew J. Schultz, **David A. Kofke***

8:38 Paper 685c: Predicting the Free-Energy Landscape of Multicomponent Fluids — ***Nathan A. Mahynski**, Jeffrey R. Errington, Vincent K. Shen*

8:57 Paper 685d: A Novel Molecular Simulation Method for Liquid-Liquid Equilibria Predictions and In-Silico Screening of Desalination Solvents — ***Prashanth Chandran**, Jindal K. Shah*

9:16 Paper 685e: SSAGES: A Comprehensive Platform for Enhanced Sampling Simulations — *Hythem Sidky, Yamil J. Colón, Benjamin J. Sikora, Cody Bezik, Federico Giberti, Ashley Guo, Julian Helfferich, Xikai Jiang, Joshua Lequieu, Jiyuan Li, Joshua Moller, Michael Quevillon, Mohammad Rahimi, Hadi Ramezani-Dakhel, Vikramjit Rathee, Daniel Reid, Emre Sevgen, Vikram Thapar, Michael Webb, Justin Wozniak, Xujun Zhao, Nicola J. Ferrier, Olle G. Heinonen, Giulia Galli, François Gygi, Juan de Pablo, **Jonathan K. Whitmer***

9:35 Paper 685f: Multiscale Modeling of Multicompartment Micelle Nanoreactors — ***Connor Callaway**, Parveen Sood, Seung Soon Jang*

9:54 Paper 685g: Reaction Ensemble Monte Carlo: Applications to Ionic Liquids — ***Ryan Gotchy Mullen**, Edward J. Maginn*

10:13 Paper 685h: Temperature-Dependent Physicochemical Properties of Nitrotoluenes from Solvation Free Energies — ***Alauddin Ahmed**, Stanley I. Sandler*

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(686) Self-Assembled Biomaterials
Thursday, Nov 2, 8:00 AM
MCC, 213A/B

Esmaiel Jabbari, Chair
Rebecca Schulman, Co-Chair
Anju Gupta, Co-Chair

Sponsored by: Bionanotechnology

8:00 Paper 686a: Self-Assembled Polymer Carriers for the Oral Delivery of High–Isoelectric Point, High–Molecular Weight Protein Therapeutics — ***Matthew Miller**, Nicholas A. Peppas*

8:15 Paper 686b: Self-Assembly of ssDNA-Amphiphiles into DNA Nanotubes with Controlled Diameters and Lengths — ***Huihui Kuang**, Thomas Gartner III, Arthi Jayaraman, Efrosini Kokkoli*

8:30 Paper 686c: Hybrid Peptide- and Protein-DNA Nanostructures — ***Nicholas Stephanopoulos***

8:45 Paper 686d: Supramolecular Nanotubes by Prodrug Assembly — ***Hao Su**, Feihu Wang, Zhantong Wang, Yuzhu Wang, Xiaoyuan Chen, Honggang Cui*

9:00 Paper 686e: Amphiphilic Polypeptoids and Their Hydrophobic Interactions with Lipid Bilayers: Fundamentals and Translation to Drug Delivery Systems — *Yueheng Zhang, **Vijay T. John**, Sunting Xuan, Zahra Heidari, Marzhana Omarova, Donghui Zhang*

9:15 Paper 686f: HINT1-Regulated Supramolecular Assembly of Nucleoside Phosphoramidate Pro-Gelators — ***Harrison T. West**, Clifford M. Csizmar, Carston R. Wagner*

9:30 Paper 686g: Self-Organization and Division in Active Biopolymer Droplets — ***Kimberly L. Weirich**, Kinjal Dasbiswas, Shiladitya Banerjee, Thomas A. Witten, Suriyanarayanan Vaikuntanathan, Margaret L. Gardel*

9:45 Paper 686h: Tuning Supramolecular Structures Self-Assembled from Fusion Proteins via Time- and Temperature-Controlled Coacervate Phase — ***Yeongseon Jang**, Julie A. Champion*

10:00 Paper 686i: Protease-Triggered, Integrin-Targeted Cellular Uptake of Recombinant Protein Micelles — ***Chen Gao**, Daniel A. Hammer, Kevin B. Vargo*

10:15 Paper 686j: An Optical Near-Infrared Doxorubicin Sensor Revealed by Principal Component Analysis of Nanosensor Libraries — ***Jackson Travis Del Bonis-O'Donnell**, Sanghwa Jeong, Rebecca Pinals, Ami Thakrar, Russ Wolfinger, Markita Landry*

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(687) Templated Assembly of Inorganic Nanomaterials
Thursday, Nov 2, 8:00 AM
MCC, 209A/B

Sunho Choi, Chair
Seok-Jhin Kim, Co-Chair

Sponsored by: Inorganic Materials

8:00 Paper 687a: Templated Synthesis of Polymer-Gold Nanocomposites with Pluronic Gels — ***Srikanth Nayak**, Surya Mallapragada, Wenjie Wang, David Vaknin*

8:18 Paper 687b: Facile Synthesis of Hierarchical MFI Zeolite with Improved Catalytic Performance — ***Chao Li**, Daiqi Ye, Hongxia Xi*

8:36 Paper 687c: Predicting Surface Area in Green Synthesis of Sol-Gel Materials — ***Brian K. Peterson**, Mobae Afeworki, David C. Calabro, Quanchang Li, Simon C. Weston*

8:54 Paper 687d: Leveraging Nanoparticle Template Assembly and Interfacial Phenomenon for Multiscale Control over Polyimide-Derived Carbon Molecular Sieve Films — ***Megha Sharma**, Mark A. Snyder*

9:12 Paper 687e: Regenerable Mesoporous MgO Calcined from Metal-Organic Frameworks (MOFs) for CO_2 Capture — ***Zelong Xie**, Christopher Cogswell, Sunho Choi*

9:30 Paper 687f: Toward Rational Design of Hierarchical Beta Zeolites via Cost-Effective Approaches — *Ke Zhang, Sergio Fernandez, Michele L. Ostraat*

9:48 Paper 687g: Nanoscale Control of Homoepitaxial Growth on a Two-Dimensional Zeolite — ***Meera Shete**, Manjesh Kumar, Donghun Kim, Neel Rangnekar, Dandan Xu, Berna Topuz, Kumar Varoon Agrawal, Evguenia Karapetrova, Benjamin Stottrup, Shaeel Al-Thabaiti, Sulaiman N. Basahel, Narasimharao Katabathini, Jeffrey Rimer, Michael Tsapatsis*

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(688) Thermodynamics at the Nanoscale
Thursday, Nov 2, 8:00 AM
MCC, L100I

Amish Patel, Chair
Sapna Sarupria, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

8:00 Paper 688a: Predicting the Solubility and Diffusivity of Gases (CO_2, CH_4, H_2, Noble Gases) in Nano-Confined Interlayer Water and Bulk Water Using Molecular Dynamics Simulations — ***Greeshma Gadikota**, Ian Bourg*

8:15 Paper 688b: Simulation of Tracer Particle Diffusion in Attractive and Repulsive Glassy Matrices — *Ryan Roberts, Ryan Poling-Skutvik, Jacinta C. Conrad, **Jeremy C. Palmer***

8:30 Paper 688c: Simulations of Biomolecular Assembly Processes at Interfaces — ***Jeetain Mittal***

9:00 Paper 688d: Characterizing Protein Hydration to Inform Its Interactions — *Erte Xi, **Amish Patel***

9:15 Paper 688e: Confinement-Induced Supercriticality and Phase Equilibria of Hydrocarbons in Nanopores — *Sheng Luo, Hadi Nasrabadi, **Jodie L. Lutkenhaus***

9:30 Paper 688f: Predictive Modeling of Adsorption and Reaction Equilibria in Nanoporous Materials [Invited Talk] — ***J. Ilja Siepmann,** Evgenii Fetisov, Mansi S. Shah, Michael Tsapatsis*

10:00 Paper 688g: Nucleation of Capillary Bridges and Bubbles — ***Jerome Delhommelle**, Caroline Desgranges*

10:15 Paper 688h: Modeling Single-Component Transport in Mesoporous Membranes Under Non-Equilibrium Conditions — ***Ashutosh Rathi**, Eustathios Kikkinides, David M. Ford, Peter A. Monson*

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(689) Thermodynamics of Polymers
Thursday, Nov 2, 8:00 AM
MCC, 211B

Sangwoo Lee, Chair
Charles E. Sing, Co-Chair

Sponsored by: Polymers

8:00 Paper 689a: Thermodynamics of Charging in Weak Polyelectrolytes — ***Jonathan K. Whitmer***

8:30 Paper 689b: Thermodynamics and Kinetics of Ordered, Strongly Segregated Diblock Copolymers — ***Ronald M. Lewis III***

8:45 Paper 689c: Effect of pH on the Interaction Between Poly(vinyl alcohol) and Ice — ***Aaron A. Burkey**, Nathaniel A. Lynd*

9:00 Paper 689d: Self-Consistent Field Theory Study of Multivalent Cation Effect on Semiflexible End-Grafted Random Polyelectrolytes — ***Merina Jahan**, Mark J. Uline*

9:15 Paper 689e: The Sequence Dependence of the Persistence Length of DNA — ***Hui-Min Chuang**, Jeffrey G. Reifenberger, Han Cao, Kevin D. Dorfman*

9:30 Paper 689f: Anomalous Hydrodynamic Radius of Polyethylene Glycol Molecules in Mixed Solvents Containing a Hydrotrope — ***Xiong Zheng**, Mikhail A. Anisimov, Jan V. Sengers, Mao-Gang He*

9:45 Paper 689g: Energy Saturation: An Alternative Mechanism for the Glass Transition — ***Isaac C. Sanchez**, Sean O'Keefe*

10:00 Paper 689h: Molecular Dynamics Simulation of Polymerized Stockmayer Fluids: Effects of Chain Length and Connectivity on Saturated Dipoles near Ions — ***Issei Nakamura**, Lijun Liu*

TECHNICAL SESSIONS 2017

10:15 Paper 689i: Probing Polymer Blend Phase Diagrams via Oligomer Molecular Simulations — ***Qile Chen***, *Shuyi Xie, Timothy P. Lodge, J. Ilja Siepmann*

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(690) Unconventionals: Hydrogen and Fuel Cells
Thursday, Nov 2, 8:00 AM
MCC, 200A

Chau-Chyun Chen, Chair
Saadet Ulas Acikgoz, Co-Chair

Sponsored by:
Alternate Fuels and New Technology

8:00 Paper 690a: A Comparative Assessment of Sol-Gel and Solid-State Syntheses–Derived Redox Materials for H_2 Production via Thermochemical Water-Splitting Process — ***Vinod S. Amar***, *Rajesh V. Shende, Jan A. Puszynski*

8:25 Paper 690b: Overview of Impact of Electrode Catalyst Loadings on Thin Flexible Fuel Cell (TFFC) Performance — ***Matthew Mayer***, *Seyed Reza Mahmoodi, Ronald S. Besser*

8:50 Paper 690c: NiMo-Ceria-Zirconia Catalytic Reforming Layer for Solid Oxide Fuel Cells Running on Isooctane — ***Kai Zhao***, *Xiaoxue (Christy) Hou, Qusay Bkour, M. Grant Norton, Su Ha*

9:15 Paper 690d: Homogeneous Reaction Kinetics of Carbohydrates with Viologen Catalysts in Biofuel Cell Applications — ***Randy S. Lewis***, *Scott Carter, Meisam Bahari, Hilary Bingham, John Harb, Gerald D. Watt*

9:40 Paper 690e: Hydrogen-Fueled Micro-Fuel Cell with Microfluidic Channels on a PFSA Plane — ***Seyed Reza Mahmoodi***, *Ronald S. Besser*

10:05 Paper 690f: Design and Analysis of Tri-Generation System Powered by Seaweed Biogas — ***Ivannie Effendi***, *Peyman Fasahati, J. Jay Liu*

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(691) Water Treatment, Desalination, and Reuse IV
Thursday, Nov 2, 8:00 AM
MCC, M100H

Isabel Escobar, Co-Chair
Jamie Hestekin, Co-Chair
Lucy Camacho, Co-Chair
Meagan Mauter, Co-Chair

Sponsored by:
Membrane-Based Separations

8:00 Paper 691a: Theoretical Investigation of Power Generation by Pressure-Retarded Osmosis — ***Mingheng Li***

8:25 Paper 691b: Removal and Prevention of Biofouling in Forward-Osmosis Membrane Bioreactors — ***Derrick J. Satterfield***, *Sage R. Hiibel*

8:50 Paper 691c: Understanding the Performance of Forward-Osmosis Hollow Fiber Membranes at the Module Scale — ***Jian Ren***, *Jeffrey McCutcheon*

9:15 Paper 691d: Novel Solvents for Carbon Dioxide Capture Using Polypropylene Membrane Contactor — ***Hojun Song***, *Honggi Jeong, Jinwon Park*

9:40 Paper 691e: Understanding the Impact of Membrane Properties and Transport Phenomena on the Energy Efficiency of a Membrane Distillation Desalination System — ***Akshay Deshmukh***, *Menachem Elimelech*

10:05 Paper 691f: Development of a Multi-Stage Membrane Distillation-Electrocoagulation Process for Treatment of Hydraulic Fracturing Flowback Waters — ***S. Ranil Wickramasinghe***, *Kamyar Sardari*

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(692) Advances in Biocatalysis and Biosynthesis II: Enzyme Engineering Applications
Thursday, Nov 2, 12:30 PM
MCC, 208C/D

Bradley C. Bundy, Chair
Robert Jinkerson, Co-Chair

Sponsored by: Bioengineering

12:30 Paper 692a: A Versatile Synthetic Biology Platform for High-Throughput Structure and Activity Screening of Ribosomally Synthesized and Post-Translational Modified Peptides (RiPPs) — ***Tong Si***, *Jonathan V. Sweedler, Wilfred A. van der Donk, Huimin Zhao*

12:48 Paper 692b: Hydroclassified Combinatorial Saturation Mutagenesis for Evolving Stereoselectivity and Cosubstrate Specificity of a Diaryl Alcohol Dehydrogenase — ***Ye Ni***, *Jieyu Zhou, Guochao Xu*

1:06 Paper 692c: Facilitating Electron Channeling in a Self-Assembling Metabolon Containing Two Dehydrogenases and an NiFe Hydrogenase — ***Hui Chen,*** *Y.-H. Percival Zhang*

1:24 Paper 692d: Beyond Iron: Iridium-Containing P450 for Selective Cyclopropanations of Alkenes — *Hanna Key, Pawel Dydio,* ***Zhennan Liu***, *Douglas S. Clark, John Hartwig*

1:42 Paper 692e: Bioprospecting to Discover Keto-Aryl Reductases with Enhanced Specificity Towards Longer-Chain, Aliphatic Substrates — ***Jason T. Boock***, *Yekaterina Tarasova, Kristala L. J. Prather*

2:00 Paper 692f: Microbial Synthesis of Novel Terpenoid-Based Inhibitors — ***Edward Y. Kim***, *Jerome M. Fox*

2:18 Paper 692g: Extreme Makeover: Engineering the Thermostable Alcohol Dehydrogenase D (AdhD) Protein Scaffold for New Applications — ***Scott Banta***

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(693) Advances in Metabolic Engineering II: Value-Added Products from Renewable Feedstocks
Thursday, Nov 2, 12:30 PM
MCC, 207A/B

Jose L. Avalos, Chair
Nathan Crook, Co-Chair

Sponsored by: Bioengineering

12:30 Paper 693a: Solvent Production Using a CO_2-Fixing, Synthetic, and Syntrophic Clostridium Co-Culture — ***Kamil Charubin***, *Eleftherios Terry Papoutsakis*

12:48 Paper 693b: Engineering *E. coli* to Consume Methanol — ***Benjamin Woolston***, *Jason King, Michael Reiter, Greg Stephanopoulos*

1:06 Paper 693c: Removal of Ribosome Stalling Motifs to Improve Oxygenation of Key Intermediate in the Taxol Pathway — ***John Lazar***, *Bradley W. Biggs, Keith E. J. Tyo*

1:24 Paper 693d: Engineering Yarrowia lipolytica for the Production of Triacetic Acid Lactone — ***Kelly Markham***, *Claire Palmer, Clare Murray, Hal Alper*

1:42 Paper 693e: Engineering a Novel Omega-3 Fatty Acid Biosynthesis Pathway in *Yarrowia lipolytica* — *Difeng Gao,* ***Mark Blenner***

2:00 Paper 693f: Establishing a Novel and Efficient Biosynthetic Pathway for Anticoagulant Precursor 4-Hydroxycoumarin in Engineered *Escherichia coli* — *Xiaolin Shen, Yuheng Lin, Monika Mahajani, Jia Wang, Qipeng Yuan,* ***Yajun Yan***

2:18 Paper 693g: Metabolic Engineering and/or Synthetic Biology for Improved Biotechnological Production: Promises and Realities — ***Eleftherios Terry Papoutsakis***

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(694) Bioinspired Membranes and Membrane Processes
Thursday, Nov 2, 12:30 PM
MCC, M100H

Manish Kumar, Co-Chair
Zhongyi Jiang, Co-Chair
Ronald Michalsky, Co-Chair

Sponsored by:
Membrane-Based Separations

12:30 Paper 694a: Bioinspired Pervaporation Membranes for Dehydration of Alcohols — *Guanhua Liu, Xuanxuan Cheng, Fusheng Pan, Jing Zhao, Hong Wu,* ***Zhongyi Jiang***

12:47 Paper 694b: Permeability and Selectivity Limits of Biomimetic Desalination Membranes — ***Jay Werber***, *Menachem Elimelech*

1:04 Paper 694c: Dipole-Oriented Water Wires Confined in Artificial Chiral Membrane Channels — ***Istvan Kocsis***, *Mirco Sorci, Heather Vanselous, Samuel Murail, Staphanie Sanders, Erol Licsandru, Yves-Marie Legrand, Arie van der Lee, Marc Baaden, Poul Petersen, Mihai Barboiu,* ***Georges Belfort***

1:21 Paper 694d: Bioinspired One-Step Co-Deposition PVDF Membrane Toward Multifunctional Applications: Oil/Water Emulsions Separation and Soluble Contaminants Adsorption — *Guangfa Zhang,* ***Jingxian Jiang***, ***Qinghua Zhang***, *Xiaoli Zhan, Fengqiu Chen*

1:38 Paper 694e: Synthesis of High-Performance Biologically Inspired Nanofiltration Membranes for Water Treatment — ***Priyesh Wagh***, *Xinyi Zhang, Yinan Wei, Isabel Escobar*

1:55 Paper 694f: Artificial Water Channels: Bioinspired and Energy-Efficient Filtration Materials — ***Yuexiao Shen***, *Manish Kumar*

2:12 Paper 694g: The Development of Hydrophobic Deep Eutectic Solvents as New Extracting Agents for Furfural and 5-Hydroxymethylfurfural from Aqueous Solutions — ***Carin Dietz***, *Maaike C. Kroon, M. van Sint Annaland, Fausto Gallucci*

2:29 Paper 694h: Multiple Morphology Control of Biomacromolecule Crystallization via Hydrogel Composite Membrane-Based Platform — ***Lin Wang***, *Gaohong He, Xiaobin Jiang*

2:46 Paper 694i: Bio-Inspired Optimization of Nanochannel Geometry and Surface Chemistry to Improve Water Permeability of Track-Etched Membrane — ***Zheyi Meng***, *Marc-Olivier Coppens*

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(695) Biomass Thermal Deconstruction via Fast-Pyrolysis Biorefineries
Thursday, Nov 2, 12:30 PM
MCC, 101D

Robert C. Brown, Chair
Mark Mba Wright, Co-Chair
Magdalena Ramirez-Corredores, Co-Chair

Sponsored by:
Sustainable Biorefineries

12:30 Paper 695a: Overcoming the Challenges of Using Corn Stover as Feedstock in Autothermal Pyrolysis — ***Joseph Polin***, *Lysle Whitmer, Ryan G. Smith, Robert Brown*

12:55 Paper 695b: Development of a Kinetics Model for Autothermal Pyrolysis in a Fluidized-Bed Reactor — ***Chad Peterson,*** *Robert C. Brown*

1:20 Paper 695c: Coupling Effects of Mass Transfer and Chemical Kinetics During the Co-Pyrolysis of Cellulose and High-Density Polyethylene — ***Melisa Nallar,*** *Hsi-Wu Wong*

1:45 Paper 695d: Fast Pyrolysis of Four Different Microalgae: Apparent Kinetic Parameters Evaluation and Product Analysis — ***Ribhu Gautam***, *R. Vinu*

2:10 Paper 695e: Overcoming Lignin Agglomeration During Pyrolytic Sugar Production in a Fluidized Bed — ***Marjorie R. Rover***, *Preston A. Gable, Ryan G. Smith, Robert C. Brown*

2:35 Paper 695f: Thermochemical Methylation of Lignin to Produce High-Value Aromatic Compounds — ***Patrick A. Johnston***, *Robert C. Brown*

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(696) Biomaterials II: Platforms for Cell Encapsulation, Isolation or Diagnostics
Thursday, Nov 2, 12:30 PM
MCC, 211A

Brad Berron, Chair
Neha Kamat, Co-Chair
Silviya Petrova Zustiak, Co-Chair

Sponsored by: Biomaterials

12:30 Paper 696a: Silica-PEG Gel Encapsulation Platform for Isolation of Dormant Cancer Cells — *Julian Preciado, Hak Rae Lee, Emil Lou, Alptekin Aksan,* ***Samira M. Azarin***

12:48 Paper 696b: Biodegradable Nano-Film-Coated Self-Floating Hollow Glass Microspheres for Rapid Cell Isolation and Recovery — ***Ziye Dong***, *Caroline Ahrens, Dan Yu, Zhenya Ding, Hyuntaek Lim, Wei Li*

1:06 Paper 696c: Design of Electrohydrodynamic Sprayed Polyethylene Glycol Hydrogel Microspheres for Cell Encapsulation — *Anisa Qayyum, Era Jain, Grant Kolar, Scott A. Sell,* ***Silviya P. Zustiak***

1:24 Paper 696d: Quantum Dot-Based Biomarkers of Neuroinflammation in the Developing Brain — ***Mengying Zhang***, *Binh Dang, Kate Hildahl, Brittany Bishop, Reyn Aoki, Nicole Thompson, Vincent C. Holmberg, Elizabeth Nance*

1:42 Paper 696e: The Culprit of Gout: Triggering Factors and Formation of Monosodium Urate Monohydrate — ***Tzu-Hsuan Chen***, *Meng-Hsiu Chih, Hung-Lin Lee, Tu Lee*

2:00 Paper 696f: Efficient Preservation of Mammalian Cells at Hypothermic Temperature Using Biocompatible Microparticles — ***Lei Zhang***

2:18 Paper 696g: Fabrication of Polyethylene Glycol-Based Templated Macroporous Hydrogels for Cell Encapsulation — ***Mozhdeh Imaninezhad***, *Grant Kolar, Silviya Petrova Zustiak*

2:36 Paper 696h: A Simple One-Step Deposition of Zwitterionic Polymer for Providing Biomaterials' Antifouling Ability via Aminomalononitrile Polymerization — *Wen-Hsuan Chen, Helmut Thissen,* ***Wei-Bor Tsai***

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(697) Bionanotechnology and Micro-Scale Technologies
Thursday, Nov 2, 12:30 PM
MCC, 208A

Mathumai Kanapathipillai, Chair
Evan K. Wujcik, Co-Chair

Sponsored by:
Engineering Fundamentals in Life Science

12:30 Paper 697a: Inhibition of Bacterial Toxin Activity Using Receptor-Based Peptides — *Eric Krueger, Shannon Hayes,* ***Angela C. Brown***

12:48 Paper 697b: Novel Inclusion Complexes for Cancer Treatment: An Approach Based on Energetics Metabolism — *Sergio Sanchez Herrero,* ***Álvaro González-Garcinuño***, *Jose M. Sanchez Alvarez, Miguel A. Galán,* ***Eva Martín del Valle***

1:06 Paper 697c: Colony Formation Within Hydrogel Microdroplets–Enabled High-Throughput Yeast Colony RNA-Seq — ***Leqian Liu***, *Adam R. Abate*

1:24 Paper 697d: Microfluidic ChIP-Seq Device for Rapid and Parallel Analysis of Histone Modifications — ***Travis Murphy***, *Sai Ma, Chang Lu*

1:42 Paper 697e: Development of Autonomous Microfluidic Chemotaxis Assay Platform for Tip-Growing Plant Cell Using Cell Elongation-Assisted Capillary-Driven Flow — *Naoki Yanagisawa*

2:00 Paper 697f: High-Throughput, Single-Cell Analysis of Peptide Uptake and Deubiquitinating Enzyme Activity Using a Microfluidic Droplet Trapping Array — *Nora Safabakhsh, Manibarathi Vaithiyanathan, Seleipiri Charles, Riad Elkhanoufi, Wayne Wortmann III,* ***Adam Melvin***

2:18 Paper 697g: Protein Engineering Approaches to Dissect Specificity in Cell Signaling — ***Sivaraj Sivaramakrishnan***

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(698) Biosensors, Biodiagnosis and Bioprocess Monitoring II: Technology and Device Development
Thursday, Nov 2, 12:30 PM
MCC, 206A/B

Kevin J. Cash, Chair
Fei Wen, Co-Chair

Sponsored by: Bioengineering

12:30 Paper 698a: A Detailed Model of Electroenzymatic Glutamate Biosensors Aids Applications In Vivo — ***Mackenzie Clay***, *Harold G. Monbouquette*

12:48 Paper 698b: Role of Interfacial Charge Concentration on Biosensing by Electrolyte-Gated Transistors — ***Mathew Thomas***, *Scott White, Kevin D. Dorfman, C. Daniel Frisbie*

1:06 Paper 698c: An Inexpensive, Point-of-Care Urine Test for Bladder Cancer in Patients — ***Abhinav P. Acharya***, *Steven R. Little*

1:24 Paper 698d: A Viscosity-Based Measurement System for Pathogen Detection — ***Katherine N. Clayton***, *Taylor Moehling, Gregory D. Berglund, Dong Hoon Lee, Andrew J. Witten, Steven T. Wereley, Jacqueline C. Linnes, Tamara L. Kinzer-Ursem*

1:42 Paper 698e: Switch-Like DNA Amplification for Biomarker Detection — ***Stephanie McCalla***, *Burcu Ozay, Cara Robertus*

2:00 Paper 698f: Rapid Diagnosis and Discrimination of Healthy and Breast Cancer Tissues Using Classical and Imaging FTIR — ***Ramazan Kizil***

2:18 Paper 698g: Genetic Circuit Design — ***Christopher A. Voigt***

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(699) Catalysis for C1 Chemistry: Methane Reforming and Syngas Conversion
Thursday, Nov 2, 12:30 PM
MCC, L100D

David Hibbitts, Chair
Pedro Serna, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

12:30 Paper 699a: Confined Ni Nanoparticles in Mesoporous Silica via a Polyethyleneimine-Assisted Route and Their Catalytic Performance for Methane Dry Reforming — ***Dohyung Kang***, *Hyun Suk Lim, Jae W. Lee*

12:48 Paper 699b: Effects of Morphology and Site Proximity on Sorption-Enhanced Steam Methane Reforming Using Hybrid Ni-CaO-Based Nanofibers — ***Luke Minardi***, *Derrick Rosales, Faisal H. Alshafei, Dante Simonetti*

1:06 Paper 699c: Methane Partial Oxidation and Dry Reforming to Syngas Using the $La_{0.9}Ca_{0.1}Fe_{03-\delta}$ Mixed-Conductor — ***Georgios Dimitrakopoulos***, *Ahmed F. Ghoniem*

1:24 Paper 699d: Probing the Catalytically Active Phase of Cobalt Fischer-Tropsch Catalysts from First Principles: Predicting High-Coverage Surface Hydroxyl Conformations Under Reaction Conditions — ***Greg Collinge***, *Catherine Stampfl, Norbert Kruse, Jean-Sabin McEwen*

1:42 Paper 699e: Promoted Mixed Oxides for "Low-Temperature" Methane Partial Oxidation in Absences of Gaseous Oxidants — ***Luke Neal***, *Arya Shafiefarhood, Junshe Zhang, Fanxing Li*

2:00 Paper 699f: The Role of Water in Low-Temperature CO Conversion Using Transition Metal Oxide–Supported Noble Metal Nanoclusters: Structure, Surface Bonding and Energetics — ***Gengnan Li***, *Liang Li, Zhiyang Huang, Di Wu*

2:18 Paper 699g: A Highly Selective Route from Syngas to Ethanol: Tandem Catalysis Unconstrained by Anderson-Schulz-Flory Distribution — ***Marat Orazov***, *Thomas F. Jaramillo*

2:36 Paper 699h: Control of Metal-Support Interaction of Fe@CNTs by Surface Modification of CNT and Its Application to Direct Olefin Synthesis from Syngas — ***Zhengpai Zhang***, *Jun Zhang, Junjie Su, Xin-Chao Xu, Binbin Zha, Jing Xu, Yi-Fan Han*

(700) Catalytic Biomass Conversion to Chemicals

Thursday, Nov 2, 12:30 PM
MCC, 200A

Nurxat Nuraje, Chair
Karthikeyan K. Ramasamy, Co-Chair

Sponsored by:
Alternate Fuels and New Technology

12:30 Paper 700a: Multi-Functional Mixed Oxide Catalysis in Cascade Chemistry to Convert Ethanol to High-Value Oxygenates — ***Mond Guo***, *Michel Gray, Karthikeyan K. Ramasamy*

12:50 Paper 700b: In-Situ Catalytic Pyrolysis of Biomass Using Blast Furnace Slag as Catalyst — ***Foster A. Agblevor***, *Ville Paasikallio, Sedat H. Beis*

1:10 Paper 700c: Acetaldehyde Condensation-Cyclodehydration to Aromatics over Mg-Al Oxides — ***Marcella Lusardi***, *Klavs F. Jensen*

1:30 Paper 700d: Calibration-Free Methods for GC Quantification of Bio-Derived Chemicals — ***Charles S. Spanjers***

1:50 Paper 700e: A Novel Method of Producing Levulinic Acid at High Concentrations and Yields from Corn Stover Hydrolysate — ***Ravikumar Gogar***, *Sridhar Viamajala, Patricia Relue, Sasidhar Varanasi*

2:10 Paper 700f: Hydrodeoxygenation of Acetic Acid as a Model Compound for the Aqueous-Phase Catalytic Pyrolysis Oils — ***Hossein Jahromi***, *Foster A. Agblevor*

2:30 Paper 700g: C_5+ Ketones Synthesis from Ethanol over Mixed Metal Oxides — ***Karthikeyan K. Ramasamy***, *Mond Guo, Michel Gray, Senthil Subramaniam*

(701) Catalytic Hydrocarbon Processing II

Thursday, Nov 2, 12:30 PM
MCC, L100B

William W. Lonergan, Chair
Steven Crossley, Co-Chair
Nan Yi, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

12:30 Paper 701a: Heterogeneous, Carbon-Supported Cobalt Oxide Catalysts for the Oligomerization of Light Olefins (C_2-C_4) into Linear Olefins — ***Joseph P. Chada***, *Zhuoran Xu, Dongting Zhao, Devon C. Rosenfeld, Jessica Rogers, Ive Hermans, George W. Huber*

12:50 Paper 701b: Molecular Modelling and Simulation of Gas Oil Hydrocracking — ***Luwen Gong***, *Nan Zhang*

1:10 Paper 701c: Understanding Catalytic Impacts on Vacuum Gas Oil (VGO) Hydrotreating Using Electrospray Ionization-Ion Mobility-Mass Spectrometry (ESI-IMMS) — ***Aamena Parulkar***, *Nicholas Brunelli, Joshua A. Thompson, Bi-Zeng Zhan*

1:30 Paper 701d: Comprehensive Mathematical Modeling of Fischer-Tropsch Synthesis Within a Microreactor — ***Andrew Traverso***, *Yousef Alanazi, Justin Pommerenck, Liney Arnadottir, Goran Jovanovic, Alexandre Yokochi*

1:50 Paper 701e: Investigation into the Superior Coking Resistance of ALD-Coated, Nickel-Based Reforming Catalysts — *Anuj Prakash, Patrick Littlewood, Elodie Guyonnet, Hanif Choudhury, Shaik Afzal, Peter C. Stair,* ***Nimir Elbashir***

2:10 Paper 701f: Hydrothermal Stability of ZSM-5 Zeolite — ***Alex Maag***, *Geoffrey Tompsett, Ron Grimm, Gisele Azimi, Luis Smith, Alexander Carl, Jason Tam, Cheen Aik Ang, Michael T. Timko*

2:30 Paper 701g: Carbon Monoxide Oxidation on Nitrogen and Copper-Doped TiO_2 — ***Guoqiang Cao***, *Nan Yi*

(702) Catalytic Hydrogen Generation I: Reforming Reactions

Thursday, Nov 2, 12:30 PM
MCC, L100C

Fuat E. Celik, Chair
Christopher L. Muhich, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

12:30 Paper 702a: Nano-Engineered Ni Catalyst for Tri-Reforming of Methane — ***Sunkyu Kim***, *Bradie S. Crandall, Jochen Lauterbach, Erdem Sasmaz*

12:50 Paper 702b: Density Functional Theory Study of Dry Reforming of Methane on Pure Nickel as Well as Transition Metal Overlayer Deposited Nickel Surfaces — ***Mohammed Minhaj*** *Ghouri, Nimir O. Elbashir*

1:10 Paper 702c: A Feasibility Study of Biogas Reforming to Improve Energy Efficiency and to Reduce Nitrogen Oxide Emissions — *Sasan Dabir, Mingyuan Cao, Richard Prosser,* ***Theodore Tsotsis***

1:30 Paper 702d: Confined Nickel Nanoparticles Supported on Silica with and Without Ceria Promoter for the Partial Oxidation of Isooctane — ***Qusay Bkour***, *M. Grant Norton, Su Ha*

1:50 Paper 702e: Aqueous-Phase Reforming of Ethanol over Cobalt-Doped Bismuth Vanadate — *Melba Aguilar,* ***Corey A. Leclerc***

2:10 Paper 702f: Nickel-Based Catalysts for Aqueous-Phase Reforming of Short-Chain Alcohols — *Martina Stekrova,* ***Irene Coronado***, *Matti Reinikainen, Pekka Simell, Juha Lehtonen, Reetta Karinen*

2:30 Paper 702g: Production of Hydrogen-Rich Syngas from Steam Reforming of Acetone over Ni-Co-Mg-Al Hydrotalcite Catalysts — ***Sanchari Basu***, *Narayan C. Pradhan*

(703) Computational Catalysis V: Oxides, Zeolites, Porous Catalysts, etc.

Thursday, Nov 2, 12:30 PM
MCC, L100E

Bin Liu, Chair
N. Aaron Deskins, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

12:30 Paper 703a: Probing Topology and Reactant Effects on Hydride Transfer in Various Zeolites from First Principles — ***Thomas T. Chen***, *Matthew Neurock*

12:48 Paper 703b: Simulations of Ammonia Adsorption for the Characterization of Acid Sites in Metal-Doped Amorphous Silicates — ***Amy Jystad***, *Alessandro Biancardi, Marco Caricato*

1:06 Paper 703c: First-Principles Grand-Canonical Simulations of Water Adsorption in Proton-Exchanged Zeolites Using a Highly Parallelizable Algorithm — ***Peng Bai***, *Matthew Neurock*

1:24 Paper 703d: The Role of ABC-6 Zeolite Cavity in Methanol-to-Olefin Conversion — ***Xu Li***, *Jihong Yu, Jianwen Jiang*

1:42 Paper 703e: Understanding the C-H Activation and Dehydrogenation Mechanisms of Alkanes on Metal Oxides — ***Mudit Dixit***, *Giannis Mpourmpakis*

2:00 Paper 703f: Prediction and Screening of Product Distribution in Nanoporous Material-Catalyzed Propene Dimerization via Molecular Simulations — ***Michelle Liu***, *Berend Smit*

2:18 Paper 703g: Catalytic Hydrogenation of Carbon Dioxide in Functionalized Metal-Organic Frameworks — ***Lin Li***, *Jingyun Ye, Karl Johnson*

2:36 Paper 703h: Inorganometallic Catalyst Design: Alkane Metathesis Catalysis in Nu-1000 MOFs Functionalized with Transition Metals — ***Bo Yang***, *Kamal Sharkas, Laura Gagliardi, Donald G. Truhlar*

(704) Computational Studies of Self-Assembly

Thursday, Nov 2, 12:30 PM
MCC, L100I

Sumit Sharma, Chair
Robert A. Riggleman, Co-Chair

Sponsored by:
Thermodynamics and Transport Properties

12:30 Paper 704a: Optimizing the Formation of Solid Solutions with Colloids of Different Shapes — ***Fernando Escobedo***

12:47 Paper 704b: Programmed Assembly of Anisotropic Patchy Colloids by Nonlinear Learning and Landscape Engineering — *Andrew W. Long,* ***Andrew L. Ferguson***

1:04 Paper 704c: Evaporation-Induced Assembly of Colloidal Crystals — ***Michael P. Howard***, *Wesley F. Reinhart, Arash Nikoubashman, Athanassios Z. Panagiotopoulos*

1:21 Paper 704d: Amphiphile-Induced Reorganization of Liquid Crystals at Aqueous Interfaces — ***Hadi Ramezani-Dakhel***, *Mohammad Rahimi, Joel Pendery, Nicholas L. Abbott, Benoit Roux, Juan de Pablo*

1:38 Paper 704e: Investigating Thermodynamics and Kinetics of a β(16-22) Peptide Aggregation Using Coarse-Grained Simulations — ***Yiming Wang***, *Stefan Auer, Sergei V. Krivov, Carol K. Hall*

1:55 Paper 704f: Inverse Materials Design from Phase Transitions in Shape Space — ***Rose Cersonsky***, *Greg van Anders, Paul Dodd, Sharon C. Glotzer*

2:12 Paper 704g: Concentration Effects in Simulations of Non-Ionic and Ionic Surfactant Micellization — ***Andrew P. Santos***, *Athanassios Z. Panagiotopoulos*

2:29 Paper 704h: Self-Assembly Simulations of Stratum Corneum Lipid Mixtures — ***Timothy C. Moore***, *Christopher R. Iacovella, Remco Hartkamp, Annette L. Bunge, Clare McCabe*

2:46 Paper 704i: Self-Assembly of Multi-Flavored DNA-Functionalized Particles into Binary Superlattices — ***Hasan Zerze***, *Nathan A. Mahynski, Evan Pretti, Vincent K. Shen, Jeetain Mittal*

(705) Critical Quality Attribute Monitoring and Control in Pharmaceutical Manufacturing II

Thursday, Nov 2, 12:30 PM
MCC, 205C

Huiquan Wu, Chair
Otute Akiti, Co-Chair

Sponsored by:
Pharmaceutical Discovery, Development and Manufacturing Forum

12:30 Paper 705a: Routine Process Monitoring for Automated Clean-in-Place Systems — ***Juan C. Silva-Martinez***

12:52 Paper 705b: Scientific Considerations and Regulatory Challenges for Low-Dose Drug Manufacturing Process Monitoring and Control — ***Huiquan Wu***, *Suyang Wu, Koushik Sowrirajan, Celia N. Cruz*

1:14 Paper 705c: Frontiers of Industrial Crystallization Science and Technology — ***Junbo Gong***, *Jingkang Wang*

1:36 Paper 705d: Models for Comparative Characterization of Complex Mixture and Biological Drug Products — ***Adam Fisher***

1:58 Paper 705e: Self-Aggregation of Gabapentin Under Confinement of Primary Particle by SMPT — ***Songgu Wu***, *Junbo Gong*

2:20 Paper 705f: Feasibility of NIR Spectroscopy for Monitoring Enzymic Digestion Process of Proinsulin Producing Insulin Glargine — ***Xu Yan***, *Lei Nie, Sheng Zhang, Weiming Wang, Haibin Wang, Wenlong Li, Haibin Qu*

2:42 Paper 705g: The Benefit of Advance Process Control in OSD Continuous Manufacturing — ***Pamela Docherty***

(706) Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains II

Thursday, Nov 2, 12:30 PM
MCC, 101E

Debalina Sengupta, Chair
Fengqi You, Co-Chair
Gerardo J. Ruiz-Mercado, Co-Chair

Sponsored by:
Sustainable Energy

12:30 Paper 706a: Process Control for Sustainability and Life-Cycle Inventory (LCI) Monitoring: Application to Biomass/Coal Co-Gasification System — ***Shuyun Li***, *Gerardo J. Ruiz-Mercado, Fernando V. Lima*

12:50 Paper 706b: Changing Global Demand for Fossil-Based Electricity with Adoption of Renewables at Urban Scale — ***Elizabeth Wachs***, *Shweta Singh*

1:10 Paper 706c: Conceptual Design of a Novel Efficient Hydrogen Production Process from Natural Gas Using the Systematic "G-H" Methodology — ***Avinash Shankar Rammohan Subramanian***, *Rahul Anantharaman, Truls Gundersen*

1:30 Paper 706d: CO_2 Capture and Conversion to Chemicals via Syngas: Reactor Modeling, Process Synthesis and Optimization — ***Priyadarshini Balasubramanian***, *Ishan Bajaj, M. M. Faruque Hasan*

1:50 Paper 706e: Methods for the Design of Spatially Explicit Biofuel Supply Chains — ***Rex T. L. Ng***, *Christos T. Maravelias*

2:10 Paper 706f: Optimization-Based Design and Analysis of a Complex Energy System Using Renewable Energy Sources to the Transport Sector — ***Seulki Han***, *Jiyong Kim*

(707) Design and Optimization of Environmentally Sustainable Advanced Fossil Energy Systems

Thursday, Nov 2, 12:30 PM
MCC, 200C

Benjamin P. Omell, Chair
David C. Miller, Co-Chair
Anthony P. Burgard, Co-Chair

Sponsored by:
Advances in Fossil Energy R&D

12:30 Paper 707a: Advancing the Production of Olefins and Aromatics from Natural Gas via Methanol: Chemical Looping for Syngas Generation — ***William W. Tso***, C. Doga Demirhan, Alexander M. Niziolek, Onur Onel, Christodoulos A. Floudas, Efstratios N. Pistikopoulos

12:52 Paper 707b: Minimizing the Economic Impact of Amine Scrubbing Using High-Fidelity Modeling and Optimization — ***Michael Baldea***, *Richard Pattison, Calvin Tsay, Gary Rochelle, Matthew S. Walters, Peter T. Frailie II, Yue Zhang*

1:14 Paper 707c: Optimal Model Synthesis for Solvent-Based CO_2 Capture Systems by Simultaneously Using Multiscale Data — ***Paul Akula***, *John Eslick, Debangsu Bhattacharyya, David C. Miller*

1:36 Paper 707d: The Value of Chemical-Looping Combustion in Future Electricity Systems — ***Clara F. Heuberger***, *Matthias A. Schnellmann, Stuart A. Scott, John S. Dennis, Niall Mac Dowell*

1:58 Paper 707e: Superstructure-Based Optimization of Membrane-Based Carbon Capture Systems — ***Miguel Zamarripa***, *Olukayode Ajayi, Michael Matuszewski, David C. Miller*

2:20 Paper 707f: Bio-Energy with Carbon Capture and Storage (BECCS): Opportunities for Efficiency Improvement — ***Mai Bui***, *Mathilde Fajardy, Niall Mac Dowell*

2:40 Paper 707g: A Process Synthesis Approach to Natural Gas Liquefaction — ***Baraka Celestin Sempuga***, *Diane Hildebrandt*

(708) Development of Intermolecular Potential Models

Thursday, Nov 2, 12:30 PM
MCC, L100J

Neeraj Rai, Chair
Shuangliang Zhao Sr., Co-Chair

Sponsored by:
Thermodynamics and Transport Properties

12:30 Paper 708a: Accelerating Force Field Parameterization to Improve the Quantitative Predictability of Thermophysical Properties — ***Richard A. Messerly***, *Andrei Kazakov*

12:46 Paper 708b: Validation of Trimethylamine-N-Oxide (TMAO) Force Fields Based on Thermophysical Properties of Aqueous TMAO Solutions — ***Daniel Markthaler***, *Johannes Zeman, Jörg Baz, Jens Smiatek, Niels Hansen*

1:02 Paper 708c: Efficient Predictions of Solvent-Mediated Interactions by Classical Density Functional Theory — ***Hongguan Wu***, *Yu Li, Shuangliang Zhao Sr., Xiaohua Lu, Honglai Liu*

1:18 Paper 708d: Optimized Mie Potentials for Phase Equilibria: Application to Noble Gases, Alkanes, Alkynes and Their Mixtures — ***Mohammad Barhaghi***, *J ason R. Mick, Jeffrey J. Potoff*

1:34 Paper 708e: Evaluation of Virial Coefficients and Their Temperature Derivatives for Multibody Potential Models — ***Navneeth Gokul***, *Andrew J. Schultz, David A. Kofke, Hainam Do, Richard J. Wheatley*

1:50 Paper 708f: Prediction of Interaction Parameters for Coarse-Grained Models Using Ab-Initio Calculations — ***Jennifer A. Clark***, *Erik E. Santiso*

2:06 Paper 708g: Modifying Nonplanar Vibration Modes of Aromatic Rings in Biomolecular Modeling — ***Faramarz Joodaki***, *Lenore M. Martin, Michael L. Greenfield*

2:22 Paper 708h: A Polarizable Force Field of Inorganic Phosphates and Hydroxyapatite Based on the Classical Drude Oscillator — ***Hadi Ramezani-Dakhel***, *Hui Li, Nader Taheri Qazvini, Juan de Pablo, Benoit Roux*

2:38 Paper 708i: Using Minimal Biasing Methods in PLUMED and LAMPPS — ***Andrew White***

(709) Diffusion in Polymers

Thursday, Nov 2, 12:30 PM
MCC, 211D

Eric Davis, Chair
Joseph F. Stanzione III, Co-Chair

Sponsored by: Polymers

12:30 Paper 709a: Multicomponent Transport Models for Non-Electroneutral Solid Electrolytes — ***Charles W. Monroe***

1:00 Paper 709b: Diffusion and Sorption Phenomena of Organic Vapor Penetrants in Unmodified and Ethylenediamine Vapor-Phase Cross-Linked Matrimid Thin Films — ***John Stanford***, *Peter Pfromm, Mary Rezac*

1:15 Paper 709c: Segmental Dynamics and Water Transport in Nafion-SiO_2 Hybrid Membranes — ***Apoorv Balwani***, *Antonio Faraone, Eric M. Davis*

1:30 Paper 709d: Designing Core/Shell Metal-Organic Framework/Polymer Films as Scalable Barrier Layers for Enhanced Protection on Photovoltaics — ***Fen Qiu***, *Zhuonan Song, Jeffrey Urban*

1:45 Paper 709e: PEO-Based Semi-Interpenetrating Polymer Networks (S-IPNs) for CO_2-Selective Membranes — ***Gregory Kline***, *Qinnan Zhang, Jennifer Weidman, Ruilan Guo*

2:00 Paper 709f: An Experimental and Triple-Mode Sorption Modeling of Sorption and Diffusion in Polymers — ***Hom Sharma***, *Stephen Harley, Yunwei Sun, Elizabeth Glascoe*

2:15 Paper 709g: In-Situ Monitoring of Emergent Transport in Polymer Membranes — ***Daniel J. Miller***, *Breanna Dobyns, Bryan S. Beckingham*

2:30 Paper 709h: The Role of Chlorine Substituent in Gas Transport Properties of Polychlorotrifluoroethene (PCTFE) — ***Milad Yavari***, *Yoshi Okamoto, Haiqing Lin*

2:45 Paper 709i: Thermodynamic Model for Predicting Swelling of Poly(N-isopropyl acrylamide) Hydrogels in Solvent Mixtures — ***Sheik Tanveer,*** *Fazle Hussain, Chau-Chyun Chen*

TECHNICAL SESSIONS 2017

(710) Diffusion, Transport and Dynamics in Adsorption Systems
Thursday, Nov 2, 12:30 PM
MCC, M100E

T. Grant Glover, Chair
Ryan Lively, Co-Chair

Sponsored by:
Adsorption and Ion Exchange

12:30 Paper 710a: Adsorption and Diffusion Phenomena in Crystal Size Engineered Zif 8 MOF — *Shunsuke Tanaka,* ***Julien Cousin Saint Remi****, Gino Baron, Joeri Denayer*

12:50 Paper 710b: Development of Concentration-Swing Frequency Response Method for Mass Transfer Studies — ***Yu Wang****, Michael Strasser, Karl Strohmaier*

1:10 Paper 710c: Measurement of Mass Transfer Parameters for Rapid Pressure Swing Adsorption — ***Aaron Moran****, Mihir Patel, Orhan Talu*

1:30 Paper 710d: Kinetic Measurements on Hierarchical Zeolites Using the Zero-Length Column — *Taylor McKillop, Zhengxing Qin, Jean-Pierre Gilson, Valentin Valtchev,* ***Enzo Mangano****, Stefano Brandani*

1:50 Paper 710e: A Parametric Study of the Adsorption/Desorption Steps for an Adsorptive Reactor (AR) Intensifying the Water-Gas Shift (WGS) Reaction — ***Secgin Karagoz****, Theodore Tsotsis, Vasilios Manousiouthakis*

2:10 Paper 710f: Quantifying Sorption and Diffusion in Polymeric and Non-Polymeric Materials: Experimental Methods and High-Fidelity Modeling — ***Elizabeth Glascoe****, Yunwei Sun, Hom Sharma, Stephen Harley*

2:30 Paper 710g: Simulation of Lysozyme Concentration Profiles at Contact Lenses and Effect of Homogenous Diffusion Coefficient — *Sinem Unal, Ece Mindek, Gonca Saglam,* ***Mustafa E. Marti****, Ahmet R. Özdural*

(711) Dynamics, Reduction, and Control of Distributed Parameter Systems
Thursday, Nov 2, 12:30 PM
MCC, 103F

Panagiotis D. Christofides, Chair
Stevan Dubljevic, Co-Chair

Sponsored by:
Applied Mathematics and Numerical Analysis

12:30 Paper 711a: Observer, Filters and Moving Horizon Estimator Design for Linear Transport-Reaction Distributed Parameter Systems — ***Stevan Dubljevic****, Qingqing Xu*

12:49 Paper 711b: Model Parameterization Through Data-Mining — ***Alexander Holiday****, Yundi Jiang, Mahdi Kooshkbaghi, William Gear, Antonios Zagaris, Yannis G. Kevrekidis*

1:08 Paper 711c: Run-to-Run Control of PECVD Systems: Application to a Multiscale CFD Model of Amorphous Silicon Deposition — ***Marquis Crose****, Anh Tran, Panagiotis D. Christofides*

1:27 Paper 711d: Dynamic Actuator Scheduling in Networked Distributed Processes Using a Receding-Horizon Optimization Approach — ***Da Xue****, Nael H. El-Farra*

1:46 Paper 711e: Modified Equation-Free Control of Distributed Parameter Systems with Model Mismatch — ***Manda Yang****, Antonios Armaou*

2:05 Paper 711f: Local Dynamic Mode Decomposition with Control: Its Application to Model Predictive Control of Hydraulic Fracturing — ***Abhinav Narasingam****, Joseph Sangil Kwon*

2:24 Paper 711g: Three-Dimensional Multiscale CFD Modeling for PECVD of Amorphous Silicon Thin Films — ***Marquis Crose****, Anh Tran, Panagiotis D. Christofides*

2:43 Paper 711h: A Model Reduction Approach for Mechanistic Biochemical Network Modeling — ***Md. Shahinuzzaman****, William S. Hlavacek, Dipak Barua*

(712) Economics and Process Control
Thursday, Nov 2, 12:30 PM
MCC, 103C

Ravendra Singh, Chair
Cory Jensen, Co-Chair

Sponsored by:
Systems and Process Control

12:30 Paper 712a: Economic Nonlinear Model Predictive Control of Continuous Pharmaceuticals Manufacturing Processes — ***Michael Shoham Patrascu****, Aditya Tulsyan, Paul I. Barton*

12:49 Paper 712b: A Scheduling Perspective on the Monetary Value of Improving Process Control — ***Joseph Costandy****, Thomas F. Edgar, Michael Baldea*

1:08 Paper 712c: A Computationally Efficient Approach to Economic Model Predictive Control via Carleman Approximation — ***Yizhou Fang****, Antonios Armaou*

1:27 Paper 712d: Handling Economic and Practical Considerations in Feedback Control of Hydraulic Fracturing in Ultra-Low-Permeability Reservoirs — ***Prashanth Siddhamshetty****, Shuai Liu, Joseph Sangil Kwon, Peter P. Valkó*

1:46 Paper 712e: Integrating RTO with Stabilizing Economic MPC — ***Douglas A. Allan****, James B. Rawlings*

2:05 Paper 712f: Combining Self-Optimizing Control and Extremum-Seeking Control: Applied to Ammonia Reactor Case Study — ***Dinesh Krishnamoorthy****, Julian Straus, Sigurd Skogestad*

2:24 Paper 712g: Combining First-Principles and Empirical Modeling for Computation Time Reduction of Economic Model Predictive Control — ***Helen Durand****, Panagiotis D. Christofides*

2:43 Paper 712h: Economic Performance Improvement for Lyapunov-Based Economic Model Predictive Control Using Disturbance Probability Distributions — ***Fahad Albalawi****, Zhe Wu, Zhihao Zhang, Helen Durand, Panagiotis D. Christofides*

(713) Emulsions and Foams
Thursday, Nov 2, 12:30 PM
MCC, M100A

Stephanie Lam, Chair
Christopher L. Wirth, Co-Chair
Ning Wu, Co-Chair

Sponsored by: Interfacial Phenomena

12:30 Paper 713a: A General Route for Nanoemulsion Synthesis Using Low-Energy Methods at Constant Temperature — ***Ankur Gupta****, Abu Zayed Md. Badruddoza, Patrick S. Doyle*

12:45 Paper 713b: Advanced Emulsion-Templating of Microreactors for the Scalable Production of Semiconductor Nanowires — ***Maritza Mujica****, Michael A. Filler, Victor Breedveld, Sven H. Behrens*

1:00 Paper 713c: The Discovery of Novel Hydrophobic DES-Water Emulsions — ***Dannie J. G. P. van Osch****, Nicole M. W. van der Heijden, Jaap van Spronsen, A. Catarina C. Esteves, Remco Tuinier, Mark Vis*

1:15 Paper 713d: Controlling Foaming During Thermal Cracking: A Non-Silicon-Based Antifoaming Agent — ***Amaka Waturuocha****, Michael Volk, Glixon Mavarez Nava, Dwijen Banerjee, Keith Wisecarver*

1:30 Paper 713e: Effect of Salt on Drainage via Stratification in Micellar Foam Films — ***Subinuer Yilixiati****, Rabees Rafiq, Yiran Zhang, Vivek Sharma*

1:45 Paper 713f: Asphaltenes Adsorption at Water/Oil Interface: A Classical Surfactant Approach — ***Shaghayegh Darjani****, Fang Liu, Nelya Akhmetkhanova, Vincent Pauchard*

2:00 Paper 713g: Rapid Demulsification of Water-in-Oil Emulsions Using Silica Nanoparticles — ***Ashwin Kumar Yegya Raman****, Clint P. Aichele*

2:15 Paper 713h: Linking Adhesive Emulsions Behaviour in Microfluidic Devices to Direct-Force Measurements Between Drop Pairs — *Christopher Fewkes, Emily Jamieson, Joe Berry,* ***Raymond R. Dagastine***

2:30 Paper 713i: Interfacial Routes to Gelation in Solid-Stabilized Emulsions — *Max Kaganyuk,* ***Ali Mohraz***

2:45 Paper 713j: Predicting the Microstructure of an Interface Laden with Anisotropic Particles — *Sri Harsha Nuthalapati,* ***Christopher L. Wirth***

(714) Feedstock Logistics for Biorefineries
Thursday, Nov 2, 12:30 PM
MCC, 101B

Allison E. Ray, Chair
Chang Dou, Co-Chair

Sponsored by: Sustainable Biorefineries

12:30 Paper 714a: Insights of Biomass Recalcitrance in Populus for Biomass Valorization — ***Chang Geun Yoo****, Yongil Yang, Xianzhi Meng, Muchero Wellington, Timothy J. Tschaplinski, Gerald Tuskan, Jin-Gui Chen, Yunqiao Pu, Arthur J. Ragauskas*

12:55 Paper 714b: Evaluation of Industrial Hemp Varieties as Potential Biomass Feedstock for Biofuels and Bioproducts — ***Wenqi Li****, Lalitendu Das, David W. Williams, Hongqiang Hu, Chenlin Li, Allison E. Ray, Jian Shi*

1:20 Paper 714c: Thermochemical Conversion of Blended Herbaceous and Woody Biomass Feedstocks — ***Charles "Warren" Edmunds****, Choo Y. Hamilton, Keonhee Kim, Timothy Rials, Nicole Labbé*

1:45 Paper 714d: Feedstock Preprocessing, Fractionation, and Blending to Improve Overall Cost, Supply, and Quality Considerations for Catalyzed and Uncatalyzed Fast Pyrolysis — ***John E. Aston****, Vicki S. Thompson, Jeffrey A. Lacey, David N. Thompson*

2:10 Paper 714e: New Approach to Ammonia Pretreatment Integrates Better Feedstock Logistics with Improved Sugar Conversion — *Jian Zhang, Venkatesh Balan,* ***Leonardo da Costa Sousa***

2:35 Paper 714f: Screening Method for Selection of Biomass Feedstock and Location for Biorefineries — ***Anders Jaksland****, Maria-Ona Bertran, Rafiqul Gani, John M. Woodley*

(715) Fundamentals of Supported Catalysis II: Oxygenate Reactions
Thursday, Nov 2, 12:30 PM
MCC, L100F

Thomas J. Schwartz, Chair
Jesse Q. Bond, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

12:30 Paper 715a: Hydrogenolysis of Propionic Acid to 1-Propanol Using a Bimetallic Pd-Re/SiO_2 Catalyst — ***James D. Kammert****, Jiahan Xie, Gopinathan Sankar, Robert J. Davis*

12:50 Paper 715b: First-Principles Insight into the High Activity and Selectivity of Pd3Cu Alloys for the Guerbet Reaction — ***Yuying Song****, Lars C. Grabow*

1:10 Paper 715c: Tunable Mixed Metal Oxides for Selective Hydrogenation and Ring-Opening of Furfuryl Alcohol — ***Taylor Sulmonetti****, Bo Hu, Zach Ifkovits, Sungsik Lee, Pradeep K. Agrawal, Christopher W. Jones*

1:30 Paper 715d: Support Effects on Ethanol Dehydrogenation over Cu Catalysts — ***Sergei Hanukovich****, Phillip Christopher*

1:50 Paper 715e: A Combined Theoretical and Kinetic Assessment of C–O Bond Rupture Pathways Within 2-Methyltetrahydrofuran over Nickel Phosphide Catalyst — ***Abdulrahman S. Almithn****, Megan E. Witzke, Christian L. Coonrod, David W. Flaherty, David D. Hibbitts*

2:10 Paper 715f: Enhanced Deoxygenation on Bifunctional Pd/Al_2O_3 Modified with Phosphonate Self-Assembled Monolayers — ***Patrick D. Coan****, Michael B. Griffin, J. Will Medlin*

2:30 Paper 715g: The Activity and Stability of Molybdenum Carbide Supported on Activated Petroleum Coke in Hydrotreating Reactions — *Kevin J. Smith,* ***Haiyan Wang****, Shida Liu*

(716) Industrial Application of Computational and Numerical Approaches to Particle Flow I
Thursday, Nov 2, 12:30 PM
MCC, 200I

Lev Davydov, Chair
Jing Huang, Co-Chair

Sponsored by:
Fluidization and Fluid-Particle Systems

12:30 Paper 716a: Application of an Efficient Discrete Particle Model to Simulate an Industrial FCC Regenerator — ***Liqiang Lu****, Sofiane Benyahia*

12:49 Paper 716b: Validated Hydrodynamic CFD Model for Catalytic Fast Pyrolysis — *Neeti Kapur,* ***Bruce Adkins****, Peter Blaser, Stephen Webb*

1:08 Paper 716c: Sine-Squared Scaling of Drag Coefficient for Different Non-Spherical Particles — ***Sathish K. P. Sanjeevi****, Johan T. Padding*

1:27 Paper 716d: Predicting and Improving FCC Reactor Cyclone Performance Using CFD Techniques — ***Raj Singh****, Eusebius Gbordzoe*

1:46 Paper 716e: CFD-DEM Modeling on Exascale Computer Architectures — ***Madhava Syamlal****, Jordan M. Musser, Ann Almgren, John Bell, Christine M. Hrenya, Thomas Hauser*

2:05 Paper 716f: Hybrid Simulations of Iron Ore Reduction in Fluidized Beds — ***Simon Schneiderbauer****, Mustafa Efe Kinaci, Franz Hauzenberger, Stefan Pirker*

2:24 Paper 716g: Verification Study of Anisotropic Filtered Two-Fluid Model Closures — *Jan Hendrik Cloete, Schalk Cloete, Stefan Radl,* ***Shahriar Amini***

(717) Innovative Technologies in Pharmaceutical Discovery, Manufacturing and Delivery
Thursday, Nov 2, 12:30 PM
MCC, 204A/B

Christopher L. Burcham, Chair
Elcin Icten, Co-Chair

Sponsored by:
Pharmaceutical Discovery, Development and Manufacturing Forum

12:30 Paper 717a: Oral Formulations: Perspectives from Additive Manufacturing — ***Andrew J. Radcliffe****, Zoltan K. Nagy, Gintaras V. Reklaitis*

12:51 Paper 717b: Predicting the Free Energy of Solvation: A Hybrid QSPR Model for Organic Solute/Solvent Pairs — *Tohid Borhani, Salvador García-Muñoz, Carla Luciani, Amparo Galindo,* ***Claire S. Adjiman***

1:12 Paper 717c: In-Silico Prediction of Absolute Rates of Crystal Growth from Solution — ***Mark Joswiak****, Baron Peters, Michael F. Doherty*

1:33 Paper 717d: Mathematical Modeling and Simulation of Magnetophoresis: Application to Drug Delivery Using Magnetic Field — ***Meenesh R. Singh****, Andreas Linninger*

1:54 Break

2:15 Paper 717f: Polyalkoxylated Alcohols as Excipients for Poorly Soluble Drugs — ***Jin Zhao****, Tom Kalantar, Mladen Ladika, Keith Harris, Christopher Tucker, Michael Tulchinsky, T. C. Kuo, Joe Kiefer, Xiaoyun Chen, Robert Krystosek*

2:36 Paper 717g: 2D-Printed Product Design of Patient-Centric Dosage Forms for Adaptive Clinical Trials — ***Diogo G. Lopes****, Wen-Kai Hsiao, Miriam Wimmer-Teubenbacher, Thomas Wutscher, Amrit Paudel, Massimo Bresciani, Patrizia Ghiotti, Frédéric Eeckman, Johannes G. Khinast*

(718) Interfacial Phenomena in Electrochemical Systems
Thursday, Nov 2, 12:30 PM
MCC, M100B

Vidhya Chakrapani, Chair
Gerold A. Willing, Co-Chair
Andrew C. Hillier, Co-Chair

Sponsored by: Interfacial Phenomena

12:30 Welcoming Remarks

12:33 Paper 718a: Controlling the Polymer/Gas Interface of the Ionic Polymer Phase of a PEM Fuel Cell Catalyst Layer During Membrane Electrode Assembly Fabrication — ***Regis Dowd Jr.****, Trung Van Nguyen*

12:51 Paper 718b: Modeling the Effect of Charged Lithium-Metal Anode on Electrolyte Decomposition — ***Luis E. Camacho-Forero****, Perla B. Balbuena*

1:09 Paper 718c: Dynamic Measurement Method of the Emulsified Water Content Based on Interfacial Polarization — ***Meiyi Qing****, Huaqing Liang, Jinjun Zhang, Min Wei, Chenbo Ma*

1:27 Paper 718d: Stretchable and Soft Electroadhesion Enhanced by Liquid-Metal Subsurface Microstructures — ***Sungjune Park****, Jun Shintake, Ishan Joshipura, Michael D. Dickey*

1:45 Paper 718e: Giant Electret Polarization in Electrochemically Deposited Hydroxyapatite Ceramic Coatings — ***Matthew Yates****, Xuefei Zhang, Wanaruk Chaimayo, Benjamin Miller*

2:03 Paper 718f: Electrochemical Charging of CdSe Quantum Dots: Effects of Adsorption Versus Intercalation — *Ajinkya Puntambekar, Qi Wang,* ***Vidhya Chakrapani***

2:21 Paper 718g: Microstructured Conducting Polymer Swabs for Enhanced Trace Explosive Detection — ***Jennifer S. Laster****, Bryan W. Boudouris, Stephen P. Beaudoin*

2:39 Paper 718h: Atomistic Modeling of Solvent Decomposition in Magnesium Batteries — ***Jeffrey S. Lowe****, Donald J. Siegel*

(719) Lithium and Beyond: Fundamental Advances in High-Performance Batteries II
Thursday, Nov 2, 12:30 PM
MCC, M100C

Paul Kohl, Chair
John Staser, Co-Chair
Nian Liu, Co-Chair

Sponsored by:
Electrochemical Fundamentals

12:30 Paper 719a: Multivalent Metal/Sulfur Chemistries for High–Energy Density Rechargeable Batteries — ***Tao Gao****, Chunsheng Wang*

12:50 Paper 719b: Understanding the Reduction Reaction Mechanisms of Sulfur-Based Cathodes: A Theoretical Approach from DFT and ReaxFF Molecular Dynamics — ***Saul Perez*** *Beltran, Perla B. Balbuena*

1:10 Paper 719c: Reversible Aluminum Intercalation in Transition Metal Sulfides — ***Linxiao Geng****, Juchen Guo*

1:30 Paper 719d: Highly Structured Titanium Nitride as Novel Cathode Materials of Lithium-Sulfur Batteries — ***Wenduo Zeng****, Mark Cheng, Simon Ng*

1:50 Break

2:00 Paper 719e: Elucidating the Solvation Structure and Dynamics of Lithium Polysulfides Using Coupled High-Throughput Simulations and Experiments — ***Nav Nidhi Rajput****, Vijayakumar Murugesan, Karl Mueller, Kristin Persson*

2:20 Paper 719f: Solvation Structure and Behavior of Lithium Polysulfide Species in Electrolytes of Lithium-Sulfur Batteries — ***Ethan P. Kamphaus****, Perla B. Balbuena*

2:40 Paper 719g: Design-Stable Room-Temperature Metal-Sulfur Batteries — ***Shuya Wei***, *Lynden A. Archer*

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(720) Materials Science in Pharmaceutical Process Development II
Thursday, Nov 2, 12:30 PM
MCC, 205D

Jason Mustakis, Chair
Lei Zhu, Co-Chair

Sponsored by:
Pharmaceutical Discovery, Development and Manufacturing Forum

12:30 Paper 720a: Using a Focused Beam Reflectance Measurement (FBRM) Probe to Characterize Tablet Disintegration Behavior as a Function of Drug Product Processing Conditions — ***Catherine Metzler***, *Michael Waldo, Joseph W. Bullard, Katie McCarty, Martha Do*

12:52 Paper 720b: Finding a Surrogate Material to an Expensive API by Applying a Multivariate Analysis on a Material Database — ***M. Sebastian Escotet-Espinoza***, *Gerardo Callegari, Marianthi Ierapetritou, Fernando Muzzio*

1:14 Paper 720c: Statistical Evaluation of Modeling Approaches of Drug Release Profiles for HPMC Matrix Tablets — *Wenzhao Yang*, ***Jin Zhao***, *Jaime Curtis-Fisk, Karen Balwinski, True Rogers, Shrikant Khot*

1:36 Paper 720d: Multivariate Data Analysis of Raw Material Properties from Pharmaceutical Powders for Predicting Compaction Behavior Using Finite Element Method — ***Jens Dhondt***, *Ashish Kumar, Bernd Van Snick, Johny Bertels, Didier Klingeleers, Chris Vervaet, Thomas De Beer*

1:58 Paper 720e: Simulation of Particle Dissolution Using the Phase-Field Approach — ***Dominik Sleziona,*** *David R. Ely, Markus Thommes*

2:20 Paper 720f: Optimization of a Low-Dose Dosator Capsule Filling Process for Dry Powder Inhalation (DPI) Applications Using In-Line PAT Approaches — ***Sandra Stranzinger***, *Eva Faulhammer, Otto Scheibelhofer, Vittorio Calzolari, Stefano Biserni, Amrit Paudel, Johannes G. Khinast*

2:42 Paper 720g: How Do Crystal Specifications Influence Pharmaceutical Tablets? — ***Nastaran Ghazi***, *Zhanjie Liu, Zhiwei Cao, Chinmay Bhat, San Kiang, Alberto Cuitino*

(721) Mechanics and Structure in Polymers
Thursday, Nov 2, 12:30 PM
MCC, 211B

Erich Bain, Chair
Santanu Kundu, Co-Chair

Sponsored by: Polymers

12:30 Paper 721a: Nanostructure-Driven Fatigue Resistance and Dynamic Recovery in Thermoplastic Elastomer Hydrogel Networks — ***Travis S. Bailey***

1:00 Paper 721b: Interfacial Crystallization of Polyolefins: An Improved Outlook for Polymer Blends — ***Alex M. Jordan***, *Kyungtae Kim, Frank S. Bates, Shaffiq Jaffer, Olivier Lhost, Christopher W. Macosko*

1:15 Paper 721c: Ultra-Stable Amorphous Teflon: Extreme Fictive Temperature Reduction as a Means to Probe Sub-Tg Dynamics — ***Gregory B. McKenna***, *Heedong Yoon, Yung P. Koh, Sindee L. Simon*

1:30 Paper 721d: Influence of Structure and Dynamics in Matrix-Free Polymer-Grafted Nanocomposite Membranes — ***Eileen Buenning***, *Sanat K. Kumar, Christopher J. Durning, Connor Bilchak, Brian C. Benicewicz, Dimitris Vlassopoulos*

1:45 Paper 721e: Role of Interfacial Adhesion in Rate-Dependent Deformation and Failure of Model Ring-Opening Metathesis Polymer (ROMP)–Filled Composites — ***Erich Bain***, *Daniel B. Knorr Jr., Joseph Lenhart*

2:00 Paper 721f: Mechanically Ductile and Stiff, Triazole-Based Glassy Photopolymer Network — ***Han Byul Song***, *Austin Baranek, Christopher N. Bowman*

2:15 Paper 721g: Controlled Topology Toughening Epoxy via Incorporation of Partially Reacted Substructures — ***Jian Gao***

2:30 Paper 721h: Thermoplastic Polydimethylsiloxane Realized by Hydrogen-Bond Networks Through L-Phenylalanine Terminals — ***Shunsuke Tazawa***, *Atsushi Shimojima, Tomoki Maeda, Atsushi Hotta*

2:45 Paper 721i: In-Vitro and -Silico Characterization of Grafted Hydrophobic Brush Membranes — ***John J. Keating***, *Mirco Sorci, Angelo Setaro, Patrick T. Underhill, Georges Belfort*

(722) Membrane Formation
Thursday, Nov 2, 12:30 PM
MCC, M100I

Neal Chung, Co-Chair
Yan Wang, Co-Chair
Ngoc Bui, Co-Chair
Dibakar Bhattacharyya, Co-Chair

Sponsored by:
Membrane-Based Separations

12:30 Paper 722a: Thermally and Chemically Treated Polyacrylonitrile Hollow Fiber Membranes for Organic Solvent Nanofiltration — *Hui Min Tham, Kai Yu Wang, Dan Hua, Susilo Japip,* ***Neal Chung***

12:48 Paper 722b: 3D Printing Polyamide Films: An Additive Approach to Making Thin-Film Composite Membranes with Tunable Thickness and Roughness — *Maqsud R. Chowdhury,* ***Jeffrey R. McCutcheon***

1:06 Paper 722c: Preparation of Porous SiC Ceramic Supports with Enhanced Air Purification Performance by Recycling of NaA Zeolite Residue — ***Zhaoxiang Zhong***, *Yi Yang, Feng Han, Weihong Xing*

1:24 Paper 722d: Graphene Oxide Membranes: Synthesis, Behavior in Organic Solvent and Application in Environmental Remediation of Toxic Organic Compounds — ***Ashish Aher***, *Mainak Majumder, Dibakar Bhattacharyya*

1:42 Paper 722e: Pilot-Scale Study of Zeolite-Y/Polyethersulfone Substrate for Composite Membrane Fabrication in CO_2 Separation — ***Dongzhu Wu***, *Yang Han, Lin Zhao, Witopo Salim, Varun Vakharia, W. S. Winston Ho*

2:00 Paper 722f: Preparation of ZIF-8 Membranes Supported on Polymer Hollow Fibers Using Microwave-Assisted Seeding and Secondary Growth — ***Moon Joo Lee***, *Mohamad Hamid, Jongmyeong Lee, Ju Sung Kim, Young Moo Lee, Hae-Kwon Jeong*

2:18 Paper 722g: Perovskite Hollow Fibers Fabrication via a Novel One-Step Thermal Processing — *Jiawei Zhu,* ***Guangru Zhang***, *Wanqin Jin*

2:36 Paper 722h: Design of High-Efficiency PVDF-PEG Hollow Fibers for Air Filtration of Ultrafine Particles — ***Liang-Yi Wang***, *Wai Fen Yong, Liya E. Yu, Neal Chung*

(723) Mixing and Segregation of Particulate Systems II
Thursday, Nov 2, 12:30 PM
MCC, 200J

Yi Fan, Chair
Joseph J. McCarthy, Co-Chair

Sponsored by:
Solids Flow, Handling and Processing

12:30 Paper 723a: Particle Motion in Vertical-Bladed Mixers — ***Humair Nadeem***, *Theodore J. Heindel*

12:49 Paper 723b: Establishing Continuum Model Segregation Parameters for Practical Particle Mixtures — ***Alexander M. Fry***, *Vidyapati Vidyapati, John P. Hecht, Paul B. Umbanhowar, Julio M. Ottino, Richard M. Lueptow*

1:08 Paper 723c: Segregation of Spherical and Non-Spherical Particles in DEM Simulations — ***Ryan P. Jones***, *Paul B. Umbanhowar, Richard M. Lueptow*

1:27 Paper 723d: Experimental Investigation of Residence Time Distribution of Free-Flowing Particles in a Lab-Scale Cylindrical Silo — *Faisal Manaf, Luke Fullard,* ***Clive Davies***

1:46 Paper 723e: Numerical Analysis of Powder Mixing Dynamics in a Ribbon Mixer — ***Alvaro Janda***, *Carlos Labra*

2:05 Paper 723f: Effect of Material Properties on the Mass Hold-Up Dynamics and Residence Time Distribution in Continuous Powder Blenders — ***M. Sebastian Escotet-Espinoza***, *Sarang Oka, Sara Mogthadernejad, Andrés D. Román-Ospino, Fernando J. Muzzio, Marianthi Ierapetritou*

2:24 Paper 723g: Solids Mixing Studies in Fluidized Beds Using Fluorescent Tracer Technique — ***Shyam Sundaram***, *S. B. Reddy Karri, Ray Cocco, Ted Knowlton*

2:43 Paper 723h: Continuum Modeling of Segregation for Polydisperse Granular Materials in Bounded Heap Flow — ***Zhekai Deng***, *Paul B. Umbanhowar, Julio M. Ottino, Richard M. Lueptow*

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(724) Modeling, Control, and Optimization of Energy Systems I
Thursday, Nov 2, 12:30 PM
MCC, 103D

Alexander W. Dowling, Chair
Edward P. Gatzke, Co-Chair

Sponsored by:
Systems and Process Control

12:30 Paper 724a: Economic Optimization of Large-Scale Embedded Battery Applications — ***Nishith R. Patel***, *James B. Rawlings*

12:49 Paper 724b: Stochastic Model Predictive Control for Battery Systems — ***Ranjeet Kumar***, *Victor M. Zavala*

1:08 Paper 724c: High-Fidelity Dynamic Simulation of Integrated Process, Control and Electrical Systems — ***Abhilash Nair***

1:27 Paper 724d: A Supervisory Predictive Control System for Solar-Load Balancing: Application to Building Energy Management — ***James Allen***, *Nael H. El-Farra*

1:46 Paper 724e: Maximizing the Output of a Solar and Natural Gas Hybrid Power Plant Using Real-Time Optimization — ***Khalid Rashid***, *Kody M. Powell*

2:05 Paper 724f: Dynamic Simulation and Optimization of Power Plants Operating at Transient Electricity Demand and Carbon Footprint Constraints — ***Chen Chen***, *George M. Bollas*

2:24 Paper 724g: Comparison in Dynamic Response of Energy-Storing Cryogenic and Chemical Absorption Carbon Capture Systems to Electricity Demand — ***Seyed Mostafa Safdarnejad***, *William Strahl, John D. Hedengren, Larry L. Baxter*

2:43 Paper 724h: Implications of Heat Integration in Energy Savings During Heat Treating of Steel — ***Hari S. Ganesh***, *Thomas F. Edgar, Michael Baldea*

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(725) MOFs, COFs, and Porous Polymer Materials I: Synthesis
Thursday, Nov 2, 12:30 PM
MCC, 209A/B

Kumar Varoon Agrawal, Chair
Yongchul G. Chung, Co-Chair
Basudeb Saha, Co-Chair

Sponsored by: Inorganic Materials

12:30 Paper 725a: Direct Synthesis and Morphology Control of Metal-Organic Framework Nanosheets — ***Feng Xue***, *Prashant Kumar, Wenqian Xu, Michael Tsapatsis*

12:49 Paper 725b: Mixed-Linker MOF Synthesis and Remediation of Acid-Gas Degradation Using Linker-Exchange Techniques — ***Krishna Chandran Jayachandrababu***, *Souryadeep Bhattacharyya, David Sholl, Sankar Nair*

1:08 Paper 725c: Rapid Microwave-Assisted Synthesis of Hybrid Zeolitic-Imidazolate Frameworks with Mixed Metals and Mixed Linkers — ***Febrian Hillman***, *John Zimmerman, Seung-Min Paek, Mohamad Hamid, Woo Lim, Hae-kwon Jeong*

1:27 Paper 725d: Micro-, Meso-, and Macro-Scale Defects in Porous Organic Cages — ***Guanghui Zhu***, *Christopher W. Jones, Ryan P. Lively*

1:46 Paper 725e: Computational Studies of the Enhanced Acidity of Defect MOF 808: The Effect of Activation Process — ***Carolina Ardila-Suárez***, *Saul Perez Beltran, Gustavo Ramirez-Caballero, Perla B. Balbuena*

2:05 Paper 725f: Crystallization Process Development of Metal-Organic Frameworks by Linking Secondary Building Units, Lattice Nucleation and Luminescence: The Insight into Reproducibility — ***Tu Lee***, *Yun Hsuan Chang, Hung-Lin Lee*

2:24 Paper 725g: Fast Mechano-Chemical Synthesis N-Doped UiO-66 with Dopamine to Enhance Chlorobenzene Competitive Adsorption Under Humid Air — ***Zhenxia Zhao***, *Peng Hu, Zhongxing Zhao*

2:43 Paper 725h: High-Yield Synthesis of ZIF-8 Nanoparticles Using Stoichiometric Reactants in a Jet-Mixing Reactor — ***Aamena Parulkar***, *Pinaki Ranadive, Nicholas Brunelli*

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(726) Multiscale and Coarse-Grained Modeling of Polymers
Thursday, Nov 2, 12:30 PM
MCC, 211C

Ahmed Ismail, Chair
Robert A. Riggleman, Co-Chair

Sponsored by: Polymers

12:30 Paper 726a: Polymer Semiflexibility Induces Non-Universal Phase Transitions in Block Copolymers — *Shifan Mao, Quinn MacPherson,* ***Andrew J. Spakowitz***

1:00 Paper 726b: A Strongly Coarse-Grained, Charge-Fluctuating Model for Polyelectrolytes — ***Nicholas Jackson***, *Marcel Langenberg, Marcus Muller, Juan De Pablo*

1:15 Paper 726c: Development of New Coarse-Grained Water Models Using Particle Swarm Optimization — ***Karteek K. Bejagam***, *Samrendra Singh, Yaxin An, Carter Berry, Sanket A. Deshmukh*

1:30 Paper 726d: Comparison of Coarse-Grained Approaches in Predicting Polymer Nanocomposite Phase Behavior — ***Jason P. Koski***, *Robert C. Ferrier Jr., Nadia M. Krook, Huikuan Chao, Amalie L. Frischknecht, Russell J. Composto, Robert A. Riggleman*

1:45 Paper 726e: Unified Polymer Erosion Model — *Joel Coffel,* ***Eric Nuxoll***

2:00 Paper 726f: Development of a Fused-Sphere SAFT-γ Mie Force Field for Polymers and Application to Poly(vinyl butyral) Adsorption to Silica — ***Christopher Walker***, *Erik E. Santiso, Jan Genzer*

2:15 Paper 726g: Effects of Coarse-Graining on Simulations of Mechanical Properties of Polymers — ***Ting Ge***, *Mark Robbins*

2:30 Paper 726h: New Computational Methods for Rapid Simulation of Hydrodynamic Interactions in Polymer Solutions — ***James Swan***, *Andrew Fiore*

2:45 Paper 726i: Coarse-Grained Molecular Dynamics Simulations of PNIPAM-Grafted Graphene Systems in an Aqueous Environment — ***Carter Berry***, *Karteek K. Bejagam, Sanket A. Deshmukh*

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(727) Nanoscale Science and Engineering in Biomolecular Catalysis II
Thursday, Nov 2, 12:30 PM
MCC, 212A/B

Su Ha, Chair
Jungbae Kim, Co-Chair
Ping Wang, Co-Chair

Sponsored by: Bionanotechnology

12:30 Paper 727a: Recent Advancement in Design and Fabricating Nanostructured Enzyme Catalyst — ***Zheng Liu***

1:00 Paper 727b: Systematic Material Design for Enzymatic Biofuel Cells — ***Takanori Tamaki***

1:30 Break

1:40 Paper 727c: Controlled Assembly of Functional Hydrogel Biomaterials with Precisely Patterned Nanostructures — ***Samuel Lim***, *Dominic J. Glover, Francois Carruzzo, Gi Ahn Jung, Douglas S. Clark*

2:00 Paper 727d: Optimizing a Porous Calcium-Phosphate Supraparticle for Enzyme Immobilization — ***Adam A. Caparco***, *Andreas S. Bommarius, Julie A. Champion*

2:20 Paper 727e: Immobilization and Stabilization of Carbonic Anhydrase into Magnetic Mesoporous Silica via Crosslinked Chitosan Coating — ***Inseon Lee***, *Kie Moon Woo, Sung-Gil Hong, Jinwoo Lee, Jungbae Kim*

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(728) Nanostructured and Self-Assembled Polymer Membranes
Thursday, Nov 2, 12:30 PM
MCC, M100J

William Phillip, Co-Chair
Ayse Asatekin, Co-Chair
Lucy Camacho, Co-Chair

Sponsored by:
Membrane-Based Separations

12:30 Paper 728a: Understanding the Effect of Nanoscopic Pore Structure on Transport in Lyotropic Liquid-Crystal Membranes — ***Benjamin J. Coscia***, *Michael Shirts*

12:50 Paper 728b: Understanding the Formation Pathways of Triblock Terpolymer Membranes — ***Katherine P. Barteau***, *Sarah A. Hesse, Peter A. Beaucage, Ulrich Wiesner*

1:10 Paper 728c: Block Polymer Hollow Fiber Membranes Functionalized with Nanoconfined Polyelectrolyte Brushes Achieve Sub-Nanometer Selectivity — ***Yizhou Zhang***, *Ryan Mulvenna, Siyi Qu, Bryan W. Boudouris, William Phillip*

1:30 Paper 728d: Polymer Nanofilms with Engineered Microporosity by Interfacial Polymerisation for Molecular Separations in Organic Solvent — ***A. G. Livingston***, *Tianyin Liu, Qilei Song, Maria F. Jimenez Solomon, Kim E. Jelfs, Marta Munoz-Ibanez*

1:50 Paper 728e: Zwitterionic Copolymer Self-Assembly for Extremely Fouling-Resistant, High-Flux Membranes with ~1 Nm Pore Size: Understanding Zwitterion Chemistry and Increasing Permeance — ***Ayse Asatekin***

2:10 Paper 728f: Nanostructured Polysulfone-Based Block Copolymer Membranes — ***Yihui Xie***, *Burhannudin Sutisna, Nicolas Moreno, Victor M. Calo, Hong Cheng, Peiying Hong, Rachid Sougrat, Ali Reza Behzad, Suzana P. Nunes*

2:30 Paper 728g: Modeling the Effects of Mass Transfer on Microstructure Formation in Phase-Inversion Membranes — ***Douglas Tree***, *Lucas Francisco Dos Santos, Glenn H. Fredrickson*

(729) Nanostructured Biomimetic and Biohybrid Materials and Devices

Thursday, Nov 2, 12:30 PM
MCC, 213A/B

Cerasela Zoica Dinu, Chair
Ardemis A. Boghossian, Co-Chair
Markita Landry, Co-Chair

Sponsored by: Bionanotechnology

12:30 Paper 729a: Peptide-Appended Hybrid[4]Arenes Are Artificial Water Channels with High Permeability and Selectivity — ***Woochul Song***, *Yuexiao Shen, Junli Hou, Manish Kumar*

12:48 Paper 729b: Highly Permeable and Selective Bioinspired Membranes Made by Membrane-Protein 2D Crystals — ***Yuexiao Shen***, *Woochul Song, Siyi Qu, William A. Phillip, Manish Kumar*

1:06 Paper 729c: Enzyme-Cleavable Peptide Amphiphiles Enhance Intracellular Delivery — ***Handan Acar***, *Nathan Donahue, James L. LaBelle, Matthew V. Tirrell*

1:24 Paper 729d: Electroactive Silk Biomimetic Composites as Flexible Electrochemical Sensors — ***Ramendra Pal***, *Vamsi K. Yadavalli*

1:42 Paper 729e: Towards Engineering Smart Nanosensors: Effects of Polymer Wrapping on Single-Walled Carbon Nanotube Photoluminescence — ***Anush Chiappino Pepe***, *Vitalijs Zubkovs, Aranya Goswami, Benjamin Lambert, Justyna Kupis-Rozmysłowicz, Dejan Djokic, Jean-Nicolas Longchamp, Ardemis A. Boghossian*

2:00 Paper 729f: Construction of Biomimetic Photocathodes Using Photosystem I-Proteoliposomes Supported on Substrates — ***Hanieh Niroomand***, *Ravi Pamu, Dibyendu Mukherjee, Bamin Khomami*

2:18 Paper 729g: Plasmonic Gel-Based Nanosensor for Colorimetric Dose Response in Proton Beam Therapy — ***Karthik Pushpavanam***, *Sahil Inamdar, Jarrod Lentz, Martin Bues, Aman Anand, Kaushal Rege*

2:36 Paper 729h: Laser-Activated Tissue-Integrating Sutures for Rapid Closure of Soft Tissue Wounds — ***Russell Urie***, *Deepanjan Ghosh, Tanner Flake, Jerry Crum, Jacquelyn Kilbourne, Kaushal Rege*

(730) NH_3 Fuel Synthesis II

Thursday, Nov 2, 12:30 PM
MCC, 101F/G

Sponsored by:
NH_3 Energy+ — Enabling Optimized, Sustainable Energy and Agriculture

12:30 Paper 730a: Design Optimization of a Distributed Ammonia Generation System — ***Matthew J. Palys***, *Alon McCormick, Prodromos Daoutidis*

12:48 Paper 730b: Exploring Peptide-Bound Catalysts for Electrochemical Ammonia Generation — *Charles Loney, Ashley Graybill, Cheyan Xu, Prashant Acharya, David Suttmiller, Luke Wiles, Katherine Ayers, Wayne Gellett, Lauren F. Greenlee,* ***Julie N. Renner***

1:06 Paper 730c: Nitride-Based Step Catalysis for Ammonia Synthesis at Atmospheric Pressure — ***Peter Pfromm***, *Michael G. Heidlage, Bin Liu, Nannan Shan, Viktor Chikan, Hongfu Luo, Nate Flesher*

1:24 Paper 730d: Dense Metallic Membrane Reactor Synthesis of Ammonia at Moderate Conditions and Low Cost — ***Thomas F. Fuerst***, *Sean T. B. Lundin, Zhenyu Zhang, Simona Liguori, J. Douglas Way, Colin A. Wolden*

1:42 Paper 730e: Our Iowa Renewable Hydrogen and Ammonia Generation System — ***Jay Schmuecker,*** *David Toyne*

2:00 Paper 730f: Process Synthesis and Global Optimization of Novel Ammonia Production Processes — ***C. Doga Demirhan***, *William W. Tso, Efstratios N. Pistikopoulos*

2:18 Paper 730g: Screening Binary Redox Pairs for Solar Thermochemical Ammonia Synthesis Using Machine-Learned Predictions of Gibbs Formation Energies at Finite Temperatures — ***Christopher J. Bartel***, *John R. Rumptz, Aaron M. Holder, Alan W. Weimer, Charles B. Musgrave*

2:36 Paper 730h: Solid Oxide Cell–Enabled Ammonia Synthesis and Ammonia-Based Power Production — ***John B. Hansen***

(731) Novel Nanoparticles and Nanostructured Materials for Catalysis — Synthesis and Processing

Thursday, Nov 2, 12:30 PM
MCC, 200H

J. Ruud van Ommen, Chair
Changsheng Su, Co-Chair

Sponsored by: Nanoparticles

12:30 Paper 731a: ALD-Modified Au-Based Catalysts for Propylene Epoxidation — *Zheng Lu, Zili Wu, C. Heath Turner,* ***Yu Lei***

12:50 Paper 731b: "Core–Shell" Nanostructured Supported Size-Selective Catalysts Prepared by Molecular Layer Deposition — ***Zeyu Shang***, *Xinhua Liang*

1:10 Paper 731c: Novel ALD-Formed Cobalt/Alumina Nanostructures Active for Fischer-Tropsch Synthesis — ***Jacob M. Clary***, *Staci A. Van Norman, Dong Su, Eric A. Stach, John L. Falconer, Charles B. Musgrave, Alan W. Weimer*

1:30 Paper 731d: Controlled Production of Nanostructured Noble-Metal Catalysts Using Atomic Layer Deposition — *Fabio Grillo, Hao Bui, Jacob A. Moulijn, Michiel Kreutzer,* ***J. Ruud van Ommen***

1:50 Paper 731e: Controlled Deposition of Metal Oxide Layers by Non-Hydrolytic Sol-Gel for Tailored Acid Sites Generation and Beyond — ***Florent Héroguel***, *Luca Silvioli, Yuan-Peng Du, Jeremy S. Luterbacher*

2:10 Paper 731f: Enhanced Hydrothermal Stability of Phosphonate-Coated Al_2O_3-Supported Catalysts — ***Timothy Van Cleve***, *Devon Underhill, J. Will Medlin*

2:30 Paper 731g: Catalytic Activity of Porphyrin-Supported Iron Oxide Clusters for Methane Oxidation — ***Melissa Barona***, *Omar K. Farha, Joseph T. Hupp, Randall Q. Snurr*

(732) Omics and High-Throughput Technologies

Thursday, Nov 2, 12:30 PM
MCC, 208B

Hung-Jen Wu, Chair
Leonidas Bleris, Co-Chair

Sponsored by:
Engineering Fundamentals in Life Science

12:30 Paper 732a: Identifying Molecular Targets of Drugs Using an Integrative Network Analysis of Protein-Protein, Protein-DNA and Transcriptomics Data — ***Heeju Noh***, ***Rudiyanto Gunawan***

12:48 Paper 732b: Integrative Omics Analysis of Cancer Protein Secretion — ***Jonathan L. Robinson***, *Jens Nielsen*

1:06 Paper 732c: A Cybernetic Approach to Modeling Lipid Metabolism in Mammalian Cells — ***Lina Aboulmouna***, *Frank T. DeVilbiss, Mano R. Maurya, Shakti Gupta, Shankar Subramaniam, Doraiswami Ramkrishna*

1:24 Paper 732d: A Constraint-Based Method for Integrating Omics Datasets to Improve Flux Predictions — ***Mingyuan Tian***, *Jennifer Reed*

1:42 Paper 732e: Supported Biomembrane Microenvironments of Controlled Phase and Cholesterol Content for Gamma-Secretase Substrate Cleavage Assays — ***M. Lane Gilchrist***, *William Houlihan, Marilia Barros, Yueming Li*

2:00 Paper 732f: Continuous Microfluidic Fabrication of Synthetic Asymmetric Vesicles as Biological Membrane Model Systems — ***Sepehr Maktabi***, *Li Lu, Jeffrey W. Schertzer, Paul R. Chiarot*

2:18 Paper 732g: Understanding the Metabolic Shift of Scheffersomyces stipitis from Aerobic Growth to Oxygen-Limited Fermentation at Genome Scale — ***Matthew Hilliard***, *Thomas Jeffries, Q. Peter He, Jin Wang*

2:36 Paper 732h: Isolation and Metagenome Analysis of Single Microdroplet-Cultivated Microbes — ***Sida (Steven) Wang***, *Larry Forney, Mark A. Burns, Xiaoxia (Nina) Lin*

(733) Planning and Scheduling I

Thursday, Nov 2, 12:30 PM
MCC, 103E

Xiang Li, Chair
Pedro M. Castro, Co-Chair

Sponsored by:
Computers in Operations and Information Processing

12:30 Paper 733a: Optimal Scheduling of Multiproduct Liquid Pipelines with Reversible Flow — ***Pedro M. Castro***

12:49 Paper 733b: Combining the Strengths of Continuous and Discrete Time Representations: A General Solution Refinement Method for Discrete-Time MIP Models — ***Hojae Lee***, *Christos T. Maravelias*

1:08 Paper 733c: A New Approach for Scheduling of Operations in Scientific Services Facilities via Multi-Commodity Flow — ***Nikolaos Rakovitis***, *Jie Li, Nan Zhang*

1:27 Paper 733d: An Integrated Chemical Site Planning and Scheduling Framework: Model and Algorithm — ***Sreekanth Rajagopalan***, *Satyajith Amaran, Nick Sahinidis, Scott J. Bury*

1:46 Paper 733e: Scheduling of Distributed Chemical and Renewable Power Production with Regulated Energy Exchange — ***Andrew Allman***, *Michael Zachar, Prodromos Daoutidis*

2:05 Paper 733f: Discrete-Time Mixed-Integer Programming Models for Simultaneous Batching and Scheduling in Sequential Environments — ***Hojae Lee***, *Christos T. Maravelias*

2:24 Paper 733g: LP Reformulation to Approximate Non-Convex Blending in MILP Scheduling Problems Using Factors — ***Brenno C. Menezes***, *Jeffrey D. Kelly, Ignacio E. Grossmann*

2:43 Paper 733h: Linear Surrogate Dynamical Models for Embedding Process Dynamics in Optimal Production Scheduling Calculations — ***Morgan Kelley***, *Richard Pattison, Ross Baldick, Michael Baldea*

(734) Rational Catalyst Design II: Metal Catalysis

Thursday, Nov 2, 12:30 PM
MCC, L100A

Luke T. Roling, Chair
Timothy Van Cleve, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

12:30 Paper 734a: Trends in Formic Acid Electro-Oxidation on Pt and Pd Monolayers on Transition Metal Surfaces: A Theoretical and Experimental Study — ***Ahmed Elnabawy***, *Jeffrey Herron, Zhixiu Liang, R. R. Adzic, Manos Mavrikakis*

12:50 Paper 734b: Activity and Thermal Stability in Well-Defined Platinum/Palladium Bimetallic Catalysts for Hydrocarbon Combustion — ***Emmett Goodman***, *Luke T. Roling, Sheng Dai, Adam Hoffman, Simon R. Bare, George Graham, Xiaoqing Pan, Frank Abild-Pedersen, Matteo Cargnello*

1:10 Paper 734c: Rational Design of Supported Ni Inverse Catalysts for Hydrogenolysis — *Ruiyi Yan, Anyang Peng, Suojiang Zhang, Z. Conrad Zhang, Harold H. Kung,* ***Mayfair C. Kung***

1:30 Paper 734d: Tuning Catalyst Activity Using Self-Assembled Monolayers — ***Lucas Ellis***, *Daniel K. Schwartz, J. Will Medlin*

1:50 Paper 734e: Investigating the Effect of Alloying Sn and Pd on Direct Synthesis of H_2O_2 — ***Pranjali Priyadarshini***, *Neil M. Wilson, Jason S. Adams, David W. Flaherty*

2:10 Paper 734f: Fabrication of Supported Size-Controlled Cobalt Nanoparticles over Porous Silicon Carbide for Superior Catalytic Performance in the Fischer-Tropsch Process — ***Viacheslav Iablokov,*** *Sergei Alekseev, Svitlana V. Gryn, Norbert Kruse*

2:30 Paper 734g: Structure-Sensitive Phenol Hydrogenation on Pd Nanostructures — *S. Sreedhala,* ***Shelaka Gupta***, *Tuhin Suvra Khan, C. P. Vinod, M. Ali Haider*

(735) Semiconducting Quantum Dots I: Surface Chemistry and Assemblies

Thursday, Nov 2, 12:30 PM
MCC, 210A/B

Ayaskanta Sahu, Chair
Vincent C. Holmberg, Co-Chair

Sponsored by:
Electronics and Photonics

12:30 Paper 735a: Gel Assemblies of Colloidal Nanocrystals — *Camila Saez Cabezas, Beth A. Lindquist, Ryan B. Jadrich, Thomas M. Truskett,* ***Delia J. Milliron***

1:00 Paper 735b: Examining the Optical Effects of Chiral Carboxylic Acids Bound to the Surface of CdSe Nanoparticles — ***Mayank Puri***, *Vivian E. Ferry*

1:16 Paper 735c: Radial Elemental Distribution Analysis of Spherical Core/Shell Nanocrystals with STEM/EDX — ***Jacob Held***, *Katharine I. Hunter, Uwe R. Kortshagen, K. Andre Mkhoyan*

1:32 Break

1:42 Paper 735d: Directional Carrier Transfer in Strongly Coupled Binary Nanocrystal Superlattice Films Formed by Assembly and In-Situ Ligand Exchange at a Liquid-Air Interface — *Yaoting Wu, Siming Li, Natalie Gogotsi, Tianshuo Zhao, Blaise Fleury, Cherie R. Kagan, Christopher B. Murray,* ***Jason B. Baxter***

2:12 Paper 735e: The Effect of CdS Shell Thickness on the Complex Index of Refraction of CdSe/CdS Core/Shell Nanocrystal Films — ***Dana Dement***, *Mayank Puri, Vivian E. Ferry*

2:28 Paper 735f: Engineering the Light-Matter Interactions of Ultrasmall CdSe Quantum Dots via Modification of Surface Species for Light-Harvesting Applications — ***Megan Webster***, *Kristi Pepa, Kevin Dominguez, Vinod Menon, Gustavo Lopez, Marco J. Castaldi, Ilona Kretzschmar*

2:44 Paper 735g: Spray Deposition of Cu_2ZnSnS_4 (CZTS) Semiconductor Photo-Electrode for Solar Rechargeable Battery — ***Animesh Mondal***, *James G. Radich*

(736) Software Engineering in and for the Molecular Sciences

Thursday, Nov 2, 12:30 PM
MCC, L100H

Eric Jankowski, Chair
Coray M. Colina, Co-Chair
Frank T. Willmore, Co-Chair

Sponsored by:
Computational Molecular Science and Engineering Forum

12:30 Paper 736a: Automated Tests for Physical Validity in Molecular Dynamics and Monte Carlo Simulations — *Pascal Merz,* ***Michael R. Shirts***

12:44 Paper 736b: Recent Developments in the HOOMD Simulation Ecosystem — ***Sharon C. Glotzer***, *Jens Glaser, Joshua A. Anderson*

1:04 Paper 736c: Using Graphs to Quantify Energetic and Structural (Dis)Order in Organic Thin Films — *Alexander Hiller, Ellen Van, Matthew Jones, Eric Jankowski,* ***Olga Wodo***

1:18 Paper 736d: Interactive Extensible Molecular Simulations with Etomica — ***Andrew J. Schultz***, *Alexander D. Kofke, David A. Kofke*

1:38 Paper 736e: A General Algorithm for Efficient Reverse-Mapping of Coarse-Grained Configurations to the Atomistic Scale — ***Christian Nowak***, *Mayank Misra, Fernando Escobedo*

1:52 Paper 736f: MOSDEF: Molecular Simulation and Design Framework — *Christoph Klein, János Sallai, Andrew Z. Summers, Christopher R. Iacovella, Ákos Lédeczi, Clare McCabe,* ***Peter T. Cummings***

2:12 Paper 736g: Massively Parallel Mesoscale Hydrodynamics on Graphics Processing Units — ***Michael P. Howard***, *Athanassios Z. Panagiotopoulos, Arash Nikoubashman*

2:26 Paper 736h: Foyer: A Framework for Defining Force Field Usage Semantics and Atom-Typing Molecular Systems — *Christoph Klein, Andrew Z. Summers, Peter T. Cummings, János Sallai, Christopher R. Iacovella,* ***Clare McCabe***

2:46 Paper 736i: Using the k-d Tree Data Structure to Accelerate Monte Carlo Simulations — ***Qile Chen***, *Bai Xue, J. Ilja Siepmann*

(737) Sustainability Metrics at the Process and Product Level

Thursday, Nov 2, 12:30 PM
MCC, 102E

Larry Erickson, Chair
Urmila M. Diwekar, Co-Chair
Hong Jin, Co-Chair

Sponsored by: Sustainability

12:30 Paper 737a: Sustainability Metrics for Miscanthus in Building Materials — ***John R. Schlup***, *Larry Erickson*

12:55 Paper 737b: Environmental Life-Cycle Assessment of Peracetic Acid Application in the Pulp and Paper Industry — ***Darlene Echeverria***, *Yuan Yao, Richard Venditti, Hasan Jameel*

1:20 Paper 737c: Evaluating Indicators and Life-Cycle Inventories for Processes in Early Stages of Technical Readiness — ***Raymond L. Smith***, *Eric C. D. Tan*

1:45 Paper 737d: Estimating the Life-Cycle Impact of Chemicals from Molecular, Thermodynamic and Charge Density Information via Mixed-Integer Optimization Techniques — ***Gonzalo Guillén-Gosálbez***, *Raul Calvo-Serrano, Maria Gonzalez-Miquel*

2:10 Break

2:35 Paper 737f: Optimal Synthesis of a Heat-Integrated Mixed-Refrigerant System for Maximum Energy Savings in Chemical/Petrochemical Industries — ***Cuixia Xu***, *Jian Zhang, Qiang Xu*

(738) Thermochemical Conversion of Biomass

Thursday, Nov 2, 12:30 PM
MCC, 200E

Catherine E. Brewer, Chair
Sunkyu Park, Co-Chair

Sponsored by:
Biorefinery Technologies for Forest-Based Lignocellulosic Biomass

12:30 Welcoming Remarks

12:35 Paper 738a: Visualization Study of Dynamic Shrinkage During Biomass Pyrolysis — ***Ali Zolghadr***, *Joseph Biernacki*

12:49 Paper 738b: Effect of Feedstock and Pyrolysis Method on the Yield of Hydrotreated Refinery Intermediate — ***Richard J. French***, *Kellene A, Orton, Stephen P. Deutch, Daniel L. Carpenter, Daniel Howe, Tyler L. Westover*

1:03 Paper 738c: ZSM-5 Coating on SiC Foam Support as a Composite Catalyst for Fast Microwave-Assisted Pyrolysis of Biomass — ***Nan Zhou***, *Shiyu Liu, Yaning Zhang, Liangliang Fan, Yanling Cheng, Erik Anderson, Yunpu Wang, Paul Chen, Yuhuan Liu, Hanwu Lei, Roger Ruan*

1:17 Paper 738d: Bio-Fuel Production from Sequential Two-Step Catalytic Fast Microwave-Assisted Biomass Pyrolysis — ***Shiyu Liu***, *Yaning Zhang, Liangliang Fan, Nan Zhou, Yanling Cheng, Erik Anderson, Yunpu Wang, Paul Chen, Yuhuan Liu, Hanwu Lei, Roger Ruan*

1:31 Paper 738e: Microwave-Assisted Fast Catalytic Pyrolysis and Gasification for Solid Wastes Conversion and Utilization — ***Roger Ruan***

1:45 Paper 738f: Synthesis of Anisotropic Calcined Coke from Fast-Pyrolysis Bio-Oils — ***Yaseen Elkasabi***, *Hans Darmstadt, Akwasi A. Boateng*

1:59 Paper 738g: Thermal Conversion of Biomass into Clean Energy and Resource Using Gasification Integrated with Power Generation and Bottom Ash Reutilization — *Thawatchai Maneerung, Xian Li, Chunyu Li, Yanjun Dai,* ***Chi-Hwa Wang***

2:13 Paper 738h: Techno-Economic Feasibility of Liquid Fuel Production Using Supercritical Water Gasification of Algal Biomass — *Alireza Rahbari,* ***Mahesh Venkataraman***, *John Pye*

2:27 Paper 738i: Pyrolysis and CO_2 Gasification Kinetics of Manure-Derived Hydrochar — *M. Toufiq Reza, Kyle McGaughy,* ***Pretom Saha***

2:41 Paper 738j: Syngas Production from Sewage Sludge by Solar-Driven CO_2 Gasification — ***Xian Li***, *Chao He, Ye Shen, Yanjun Dai, Chi-Hwa Wang*

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(739) Adsorbent Materials: MOFs
Thursday, Nov 2, 3:15 PM
MCC, M100I

Bin Mu, Chair
Sasidhar Gumma, Co-Chair

Sponsored by:
Adsorption and Ion Exchange

3:15 Paper 739a: MOF Molecular Sieves to Address Challenging Gas/Vapor Separations: Present and Future — ***Youssef Belmabkhout***

3:33 Paper 739b: Understanding CO_2 in MOF-74: Dynamics and Structure of Adsorbed CO_2 with ^{13}C NMR and DFT — *Robert M. Marti,* ***Joshua D. Howe***, *Cody R. Morelock, Mark S. Conradi, David S. Sholl, Sophia E. Hayes, Krista S. Walton*

3:51 Paper 739c: Using Metal-Organic Frameworks for CO Purification: Investigation of Key Material Parameters Through a Multiscale Approach — ***Arwyn Evans***, *Ryan Luebke, Matthew Cummings, Andi Tao, Abdulmalik Ajenifuja, Martin Attfield, Flor R. Siperstein, David Fairen-Jimenez, Megan Jobson, Klaus Hellgardt, Camille Petit*

4:09 Paper 739d: Binary Adsorption of CO_2 and Water on UiO-66 MOF — *Jackson Cunningham, Mohammad I. Hossain, Tim Becker, Brooks D. Rabideau,* ***T. Grant Glover***

4:27 Paper 739e: Designing MOF-Embedded Electrospun Fibers for Adsorption Applications — ***Mitchell Armstrong***, *Bin Mu*

4:45 Paper 739f: Butanol Separation from Multicomponent Vapor Mixtures Using Zeolitic Imidazolate Frameworks — ***Souryadeep Bhattacharyya***, *Krishna Chandran Jayachandrababu, David S. Sholl, Sankar Nair*

5:03 Paper 739g: Synthesis of Water-Sensitive Metal-Organic Frameworks Within Fiber Sorbent Modules — ***Brian R. Pimentel***, *Adam W. Fultz, Kristin V. Presnell, Ryan P. Lively*

5:21 Paper 739h: A Robust Iron-Based Metal-Organic Framework PCN-250 for Adsorption Separation of C_2H_6 over C_2H_4 — *Yongwei Chen, Zhiwei Qiao, Qibin Xia, Jing Xiao, Hongxia Xi, Jian Zhou,* ***Zhong Li***

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(740) Atomistic and Molecular Modeling and Simulation of Polymers
Thursday, Nov 2, 3:15 PM
MCC, 102A

Charles E. Sing, Chair
Jonathan K. Whitmer, Co-Chair

Sponsored by: Polymers

3:15 Paper 740a: Computational Prediction and Evolutionary Design of Polymer Glass-Formation Behavior — ***David S. Simmons***, *Jui-Hsiang Hung, Venkatesh Meenakshisundaram, Tarak Kumar Patra*

3:45 Paper 740b: Domain Spacing and Phase Behavior of Salt-Doped Block Copolymers from Fluids Density Functional Theory — *Jonathan R. Brown,* ***Lisa M. Hall***

4:00 Paper 740c: Atomistic Simulations of Lamellae-Forming PS-b-P2VP — ***Yamil J. Colón***, *Weiwei Chu, Juan de Pablo*

4:15 Paper 740d: Rapid Conformational Fluctuations in a Model of Methylcellulose — ***Xiaolan Li***, *Frank S. Bates, Kevin D. Dorfman*

4:30 Paper 740e: Multi-Phase Coarse-Grained Models of Rod-Like Polymers from Iterative Boltzmann Inversion — ***Christian Nowak***, *Fernando Escobedo*

4:45 Paper 740f: Coarse-Grained Model of Exciton Dynamics on Long-Chain Conjugated Polymer System — ***Elizabeth M. Y. Lee***, *William A. Tisdale, Adam P. Willard*

5:00 Paper 740g: Molecular Simulation of Thermoplastic Polyurethanes Under Large Mechanical Deformation — ***Shuze Zhu***, *Gregory C. Rutledge*

5:15 Paper 740h: Harnessing Virtual High-Throughput Screening and Machine Learning for the Discovery of Novel High–Refractive Index Polymers — ***Johannes Hachmann***

5:30 Paper 740i: Development of Reaction Ensemble Monte Carlo (REMC) Algorithms to Study the Kinetics of Polymerization — ***Inderdip Shere***, *Ateeque Malani*

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(741) Biobased Materials: Design and Application
Thursday, Nov 2, 3:15 PM
MCC, 103C

Derek Englert, Chair
Phanourios Tamamis, Co-Chair

Sponsored by: Bioengineering

3:15 Paper 741a: Controlled Liquid-Liquid Phase Separation of Recombinant Oleosin — *Ellen H. Reed,* ***Daniel A. Hammer***

3:33 Break

3:51 Paper 741c: Evaluation of the Procedure to Obtain Chitosan-Based Gels with Potential Use as Bone Adhesive on Clinical Settings — ***Paula A. Sarmiento***, *J. German Vargas, Jairo A. Jimenez, Juan Carlos Briceño, Camila Castro, Juan Pablo Casas, Felipe Salcedo*

4:09 Paper 741d: Deep Space Drug Shielding — *Hannah Kim, Manosi Roy,* ***Sutapa Barua***

4:27 Paper 741e: Synthesis of Designer Lipids Using "Click" Chemistries — ***Danielle Konetski***, *Dawei Zhang, Austin Baranek, Tao Gong, Brady Worrell, Christopher Bowman*

4:45 Paper 741f: Loading and Mobility of RNA in Porous Silica Nanoparticles for Delivery to Insects — ***Shanshan Zhou***, *Emily Nadeau, M. Arif Khan, Bruce Webb, Stephen E. Rankin, Barbara L. Knutson*

5:03 Paper 741g: Engineering and Functionalizing Protein-Based Materials — ***Sarah Bondos***

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(742) Biomimetic Materials I: Design and Synthesis
Thursday, Nov 2, 3:15 PM
MCC, 102F

Zhiqiang Cao, Chair
Adrianne M. Rosales, Co-Chair
Nitin Agrawal, Co-Chair
Wei Li, Co-Chair

Sponsored by: Biomaterials

3:15 Paper 742a: Synthesis and Applications of Bio-Inspired Oligo TEA Peptidomimetics — ***Christopher A. Alabi***

3:51 Paper 742b: A Polyester-Based Photoluminescent Hydrogel as Extracellular Matrix Mimics — ***Xiaoyang Xu***

4:09 Paper 742c: Alginate Nanoparticle Platform for Controlled Release of Biotherapeutics — ***Julia Vela Ramirez***, *Daniela Barrios Santos, Nicholas A. Peppas*

4:27 Break

5:03 Paper 742f: Complex Bone Regeneration via Controlled Release of Simple Signaling Molecules — ***Soheila Aliakbarighavimi***, *Brittany Allen, Jessica Stromsdorfer, Jake Kramer, Ram Rao Tata, Andrew Greenwald, Bret Ulery*

5:21 Paper 742g: Biomimetic Growth of a Pathologic Biomineral in Hydrogels — ***Gopichand Mallam***, *Marina Tsianou*

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(743) Catalysis for C1 Chemistry: Forming C-C Bonds from Methane
Thursday, Nov 2, 3:15 PM
MCC, M100G

Ali A. Rownaghi, Chair
Hongfei Lin, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

3:15 Paper 743a: Exploring Ruthenium Metal-Support Dynamics for the Low-Temperature Partial Oxidation of Methane — ***Emmett Goodman***, *An-Chih Yang, Allegra A. Latimer, Liheng Wu, Frank Abild-Pedersen, Matteo Cargnello*

3:33 Paper 743b: Effect of Gold-Palladium Particle Size on Methane Oxidation Activity — ***Christopher Williams***, *James H. Carter, Nicholas F. Dummer, Robert Armstrong, David Willock, Sara Yacob, Randall J. Meyer, Stuart H. Taylor, Graham J. Hutchings*

3:51 Paper 743c: Direct Methane Conversion to Ethylene and Ethane by Oxidative Coupling in Packed-Bed and Membrane Reactors — ***Valentina Omoze Igenegbai***, *Suljo Linic*

4:09 Paper 743d: Sulfur as a Selective Soft Oxidant in the Catalytic Conversion of Methane to Ethylene over Metal Chalcogenides — ***Sagar Udyavara***, *Matthias Peter, Tobin J. Marks, Matthew Neurock*

4:27 Paper 743e: Methane Coupling in Atmospheric Pressure Corona-Discharge Microreactor — ***Adam Shareghi***, *Ian Reddick, Justin Pommerenck, Scott Harpool, Yu Miao, Yousef Alanazi, Alexandre Yokochi, Annette von Jouanne, Nick AuYeung, Goran Jovanovic*

4:45 Paper 743f: Non-Oxidative Methane Coupling Using Metal Hydrides as Hydrogen Storage Materials — ***Quan Do***, *Lars C. Grabow*

5:03 Paper 743g: Oxidative Coupling of Methane over Mixed Metal Oxides — ***Sarsani Sagar***, *Wugeng Liang, David West, Vemuri Balakotaiah*

5:21 Paper 743h: Experimental and Theoretical Investigation on Methane Dehydroaromatization Under Non-Oxidative Conditions — ***Sonit Balyan***, *Tuhin Suvra Khan, Sourabh Mishra, M. Ali Haider, K. K. Pant*

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(744) Catalytic Hydrogen Generation II: Shift and Splitting Reactions
Thursday, Nov 2, 3:15 PM
MCC, M100E

Fuat E. Celik, Chair
Ronald Michalsky, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

3:15 Paper 744a: Photocatalytic Hydrogen Generation onto Mesoporous Titania Doped with Pt — ***Fabricio Guayaquil Sosa***, *Benito Serrano, Hugo de Lasa*

3:35 Paper 744b: TiO_2 Nanoparticles by Flame Synthesis for Photocatalytic Hydrogen Evolution — *Shyang Wu, Weijing Wang, Markus Kraft,* ***Rong Xu***

3:55 Paper 744c: $Ni(OH)_2$-Decorated Jagged Pt Nanowires Have High Activities for Hydrogen Evolution Reaction — ***Kaining Duanmu***, *Mufan Li, Zipeng Zhao, Peng Li, Phillippe Sautet, Yu Huang, Xiangfeng Duan*

4:15 Paper 744d: Selective and Highly Stable H_2 Production from Formic Acid Decomposition over Graphite-Supported MoC — ***Jake T. Gray***, *Norbert Kruse, M. Grant Norton, Su Ha*

4:35 Paper 744e: Catalytic Trends for Nanoscale Catalysts from First-Principles Modeling and Tuning of Catalytic Reactivity for Fuel Production — ***Mingxia Zhou***, *Bin Liu*

4:55 Paper 744f: Sorption-Enhanced Water-Gas Shift (SE-WGS) Reaction Processes for the Production of High-Purity Hydrogen — ***Chan Hyun Lee***, *Ki Bong Lee, Hyung Chul Ham, Jonghee Han*

5:15 Paper 744g: Aldehyde-Water Shift Reaction: Comparative Investigation of Supported Metal Catalysts — ***Wei-Chung Wen***, *Levi T. Thompson*

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(745) Conversion of Biomass-Based Renewable Resources to Synthesis Gases and Pyrolysis Oils
Thursday, Nov 2, 3:15 PM
MCC, 101C

Eric C. D. Tan, Chair
Chenlin Li, Co-Chair

Sponsored by:
Sustainable Biorefineries

3:15 Paper 745a: The Selection and Optimization of Heat Carrier Materials to Maximize Liquid Yields and Heat Recovery in Auger Pyrolyzers — ***Tannon J. Daugaard***, *Mark Mba Wright*

3:40 Paper 745b: A Kinetic Study of the Fast Micro-Pyrolysis of Hybrid Poplar — ***Bethany Klemetsrud***, *Jordan Klinger, Ezra Bar Ziv, David R. Shonnard*

4:05 Paper 745c: Experimental Investigation of Tar Recycling in Biomass Gasification — ***Jia Yu***, *Haider Al-Rubaye, Joseph D. Smith*

4:30 Paper 745d: Energy and Exergy Analysis of a Mobile Autothermal Pyrolysis System for Local Biomass Conversion — ***Xing Chen***, *Huiyan Zhang, Rui Xiao*

4:55 Paper 745e: A Convolutional Neural Network Model for Biomass Gasification in Fluidized Bed — ***Mohsen Dirbaz***, *Hamid Arastoopour, Javad Abbasian*

5:20 Paper 745f: Upgrading Biomass Using Low-Temperature Plasma — ***Yu Gao***, *Necip Uner, James Meyer, Marcus Foston, Elijah Thimsen*

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(746) Critical Quality Attribute Monitoring and Control in Pharmaceutical Manufacturing III
Thursday, Nov 2, 3:15 PM
MCC, 101D

Huiquan Wu, Chair
Otute Akiti, Co-Chair

Sponsored by:
Pharmaceutical Discovery, Development and Manufacturing Forum

3:15 Paper 746a: Application of Radiometric Sensor for Inline Mass Flow Rate Monitoring and Control of a Continuous Tablet Manufacturing Line — ***Sudarshan Ganesh***, *Qinglin Su, Zoltan K. Nagy, G. V. Reklaitis*

3:40 Paper 746b: Design Space Development for the Dropping Process of a Dripping Pill with Material Attributes Represented as the Scores from Principal Component Analyses of Spectra Data — ***Xingchu Gong***, *Jichen Shen, Haibin Qu*

4:00 Paper 746c: Water Proton NMR for Noninvasive Chemical and Pharmaceutical Analysis — ***Bruce Yu***, *Marc Taraban, Yue Feng, Katharine Briggs*

4:25 Paper 746d: Monitoring the Whole Blending End-Point of An-Gong-Niu-Huang Wan Using the QbD Concept — ***Xiaona Liu***, ***Qiusheng Zheng***, ***Xiaoqing Che***, ***Zhisheng Wu***, ***Yanjiang Qiao***

4:45 Paper 746e: Steady-State Data Reconciliation of a Direct-Compression Tableting Line — ***Mariana Moreno***, *Jianfeng Liu, Sudarshan Ganesh, Qinglin Su, Nima Yazdanpanah, Thomas O'Connor, Carl Laird, Zoltan K. Nagy, Gintaras Reklaitis*

5:05 Paper 746f: Considerations for Control of Manufacturing Processes for Transdermal Systems: FDA Perspective — ***James Norman***, *Yubing Tang, Sharmista Chatterjee*

5:25 Paper 746g: Real-Time Release Testing Using a Quality Data Management Software: SIPAT — ***Pamela Docherty***

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(747) Data Mining and Machine Learning in Molecular Sciences II
Thursday, Nov 2, 3:15 PM
MCC, 103A

Johannes Hachmann, Chair
Andrew L. Ferguson, Co-Chair
Diwakar Shukla, Co-Chair

Sponsored by:
Computational Molecular Science and Engineering Forum

3:15 Paper 747a: Machine Learning for Autonomous Crystal Structure Identification — ***Wesley F. Reinhart***, *Andrew W. Long, Michael P. Howard, Andrew L. Ferguson, Athanassios Z. Panagiotopoulos*

3:27 Paper 747b: Intelligent, Autonomous Exploration of Self-Assembly Simulation Parameter Space — ***Matthew Spellings***, *Sharon C. Glotzer*

3:39 Paper 747c: Efficient Phase Diagram Sampling by Active Learning — ***Chengyu Dai***, *Isaac Bruss, Sharon C. Glotzer*

3:51 Paper 747d: A Path Entropy-Based Approach to Predict Transition Rates from Limited Information — ***Purushottam Dixit***

4:03 Paper 747e: Iterative Manifold Extension for Efficient Discovery of Transition Pathways — ***David Sroczynski***, *Juan Bello-Rivas, Hau-tieng Wu, Eliodoro Chiavazzo, Ioannis G. Kevrekidis*

4:15 Paper 747f: Learning Free-Energy Landscapes Using Artificial Neural Networks — ***Hythem Sidky***, *Jonathan K. Whitmer*

4:27 Paper 747g: QM/ML: A Hybrid Quantum-Mechanics/Machine-Learning Scheme — ***Yinjia Zhang***, *Andrew A. Peterson*

4:39 Paper 747h: Automation of an Energy Renormalization Approach for the Temperature-Transferable Coarse-Graining of Glass-Forming Polymers — *Wenjie Xia, Brian Moroz, Jack F. Douglas, Sinan Keten,* ***Frederick R. Phelan Jr.***

4:51 Paper 747i: Developing Theory and Data-Driven Benchmarks for General Coarse-Grained Mapping Operators — *Maghesree Chakraborty,* ***Andrew White***

5:03 Paper 747j: New Coarse-Grained Models of Hydrocarbons — ***Yaxin An***, *Karteek Bejagam, Sanket Deshmukh*

5:15 Paper 747k: Constrained Best-Subset Selection Methodology for the Regression of Helmholtz Energy Equations — ***Marissa Engle***, *Nick Sahinidis*

5:27 Paper 747l: Identifying Equilibrated Simulation Trajectories with Artificial Neural Networks — ***Eric Jankowski***, *Mitchell Leibowitz, Evan Miller, Michael Henry*

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(748) Developments in the Pretreatment of Lignocellulosics for Bioconversion
Thursday, Nov 2, 3:15 PM
MCC, 101A

David Hodge, Chair
David N. Thompson, Co-Chair

Sponsored by:
Sustainable Biorefineries

3:15 Paper 748a: Cellulose Pretreatment and Dissolution: Selection of Solvent and Processing Conditions — *Mohammad Ghasemi, Luz V. Vargas-Aponte, Marina Tsianou,* ***Paschalis Alexandridis***

3:36 Paper 748b: Ionic Liquids: Solvent Design for Diverse Sustainable Biomass Valorisation — *Andre M. da Costa Lopes,* ***Rafal M. Lukasik***

3:57 Paper 748c: Pretreatment of Biomass and Coal with Ionic Liquids for Advanced Fuel and Chemical Production — ***C. Luke Williams***, *Chenlin Li, Jared C. Allen, Karen M. Delezene-Briggs*

4:18 Paper 748d: In-Situ Raman Microscopy to Monitor Changes in Cellulose Crystallinity During Acid Pre-Treatment — ***Maksim Tyufekchiev***, *Geoffrey Tompsett, Michael T. Timko*

4:39 Paper 748e: Hydrochloric Acid–Pretreated Digested Carica papaya Petioles, Towards Holistic Biogas Potential Assessment Frameworks — ***Cory Jensen***, *David Olugbemide*

5:00 Paper 748f: Supercritical CO_2 Pretreatment of Wheat Straw: Hydrolysis Performance, Enzymatic Yields and Comprehensive Mass Balances — ***Ana R. C. Morais***, *Rafal M. Lukasik*

5:21 Paper 748g: Dilute Alkali Flowthrough Pretreatment of Softwood — *Libing Zhang, Yucai He,* ***Bin Yang***

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(749) Directed and Self-Assembly of Colloids
Thursday, Nov 2, 3:15 PM
MCC, M100A

Peng Jiang, Chair
Zhengdong Cheng, Co-Chair
Bhuvnesh Bharti, Co-Chair

Sponsored by:
Interfacial Phenomena

3:15 Paper 749a: Diverse Colloidal Crystals from DNA-Grafted Spheres via Self-Assembly — ***Yifan Wang***, *Ian Jenkins, James T. McGinley III, Talid Sinno, John C. Crocker*

3:30 Paper 749b: Material Design by DNA-Mediated Interactions Between Colloids — ***Runfang Mao***, *Jeetain Mittal*

3:45 Paper 749c: High-Throughput Acoustically Driven Self-Assembly of Microfluidic Colloidal Crystals — ***Meghana Akella***, *Jaime Juárez*

4:00 Paper 749d: The Role of Interaction Heterogeneity in Colloidal Crystallization — ***Ian Jenkins***, *John C. Crocker, Talid Sinno*

4:15 Paper 749e: Self-Assembly of Open Structures Using Depletion — ***Jens Glaser***, *Sharon C. Glotzer*

4:30 Paper 749f: Controlled Self-Assembly of Colloidal Discotic Liquid Crystals — ***Zhengdong Cheng***

4:45 Paper 749g: Stratification Dynamics in Drying Colloidal Mixtures — ***Michael P. Howard***, *Arash Nikoubashman, Athanassios Z. Panagiotopoulos*

5:00 Paper 749h: Theoretical and Experimental Investigation of Phase Separation in Noble Metal Nanoparticle Monolayers — ***Steven Merz***, *Zachary Farrell, Sergei Egorov, David L. Green*

5:15 Paper 749i: Bending-Induced Buckling Instabilities in Self-Assembled Elastomeric Composite Films — ***Peng Jiang,*** *Sin-Yen Leo, Zhuxiao Gu*

5:30 Paper 749j: Molecular Modeling of Microstructure, Solubilization and Micro-Emulsion of Block Copolymer Micelles by iSAFT — ***Shun Xi***, *Le Wang, Walter G. Chapman*

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(750) Fundamentals of Supported Catalysis III: Metal/Support Interactions
Thursday, Nov 2, 3:15 PM
MCC, M100F

David Hibbitts, Chair
Branko Zugic, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

3:15 Paper 750a: 2-Propanol Decomposition on TiO_x/Au/SiO_2: Probing Properties of the Interfacial Perimeter Sites — *Yi Y. (Chloe) Wu,* ***Harold H. Kung***

3:35 Paper 750b: Determining How Support pH and Hydrophilicity and Metal Particle Size Influence Activity and Product Distributions in Aqueous-Phase Reforming of Glycerol — ***Torrie Sewell***, *David A. Bruce, Rachel Getman*

3:55 Paper 750c: Measurement of the Concentration and Intrinsic Catalytic Activity of Monometallic and Interfacial Sites — *Insoo Ro, Yifei Liu, Isaias B. Aragao, Madelyn Ball, Joseph P. Chada, Canan Sener, Daniela Zanchet, James A. Dumesic,* ***George W. Huber***

4:15 Paper 750d: Furfuryl Alcohol Dehydration over Metal Oxides (TiO_2, Al_2O_3 and Nb_2O_5)–Supported WO_3 Catalysts — ***Xiaojun Chan***, *Jaeky Liu, Jaekuang Lee, Christin Abraham, Aaron Min, Taejin Kim*

4:35 Paper 750e: Support-Induced Control of Surface Composition in Bimetallic Catalytic Particles — *Bhogeswararao Seemala, Charles M. Cai, Charles E. Wyman,* ***Phillip Christopher***

4:55 Paper 750f: Nature of Molecular Interactions of Bio-Oil Derivatives on Thiolate-Coated Pd Nanoparticles — ***Lesli Mark***, *Will Medlin, Hendrik Heinz*

5:15 Paper 750g: Surface Characterization of 2D Metal-Supported Bilayer Silica and Aluminosilicates as Model Zeolites — ***Gregory S. Hutchings***, *Jin-Hao Jhang, Chao Zhou, Udo D. Schwarz, Eric I. Altman*

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(751) Industrial Application of Computational and Numerical Approaches to Particle Flow II
Thursday, Nov 2, 3:15 PM
MCC, 200I

Clay Sutton, Chair
Madhava Syamlal, Co-Chair

Sponsored by:
Fluidization and Fluid-Particle Systems

3:15 Paper 751a: Investigation of Particle Cluster Morphology in a Downflow Reactive System via Large Eddy Simulations — ***Noel A. Gómez***, *Laurien A. Vandewalle, Pieter A. Reyniers, David J. Van Cauwenberge, Alejandro Molina, Rodney O. Fox, Kevin M. Van Geem, Guy B. Marin*

3:37 Paper 751b: Numerical Simulation of an Industrial Gas-Solid Flow by the Coarse-Grain Model — ***Kazuya Takabatake***, *Mikio Sakai*

3:59 Paper 751c: Dynamic Multiscale Method for Gas-Solid Flow — *Xizhong Chen,* ***Junwu Wang***

4:21 Paper 751d: Applying Data-Driven Dimension Reduction Techniques to Constitutive Model Formulation for Gas-Particle Flows — ***Yundi Jiang***, *Ali Ozel, Mahdi Kooshkbaghi, Yannis G. Kevrekidis, Sankaran Sundaresan*

4:43 Paper 751e: Spatially Averaged Models for Dense Gas-Solid Flows — ***Simon Schneiderbauer***

5:05 Paper 751f: CFD Analysis for Boundary Effect of Particle Flow in Pipeline Manifold — ***Mohanrao Rampure***

5:27 Paper 751g: Numerical Simulations of PSRI Cold-Flow FCC Stripper Experiment with Subway Grating Baffles — ***Samuel M. Clark***, *Jeffery S. Logsdon, Allan Issangya, Ray Cocco, Peter Blaser*

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(752) Industrial Applications of Metabolic Engineering
Thursday, Nov 2, 3:15 PM
MCC, 103B

Hsien-Chung Tseng, Chair
Tong Si, Co-Chair

Sponsored by: Bioengineering

3:15 Paper 752a: Lab Automation for Industrial Biotechnology: High-Throughput Cloning for Genome-Scale Over-Expression Library Creation and Parts Assembly — ***Meng Wang***, *Haijiao Cheng, Ye Liu*

3:33 Paper 752b: Non-Growth Metabolism in Synthetic Auxotrophic Knockouts of Escherichia coli for Chemical Production — ***William Bothfeld***, *Stephen Lillington, Keith E. J. Tyo*

3:51 Paper 752c: Engineering of a Highly Efficient Escherichia coli Strain for Mevalonate Fermentation — ***Jilong Wang***, *Kechun Zhang*

4:09 Paper 752d: Enabling Glucose-Xylose Co-Utilization in Yeast Through Expression of Xylose-Specific Transporters — ***Meirong Gao,*** *Mingfeng Cao, Qianhe Su, Zengyi Shao*

4:27 Paper 752e: Deciphering the Elusive Role of Branched-Chain Amino Acid Transaminases in the Production of Branched-Chain Higher Alcohols in *Saccharomyces cerevisiae* — *Sarah Hammer,* ***Jose L. Avalos***

4:45 Paper 752f: Metabolic Engineering for Terpenoids Overproduction and Discovery — ***Tiangang Liu***, *Guangkai Bian, Tian Ma, Yichao Han, Fayin Zhu, Yujie Yuan, Anwei Hou, Shu Cheng, Zixin Deng*

5:03 Paper 752g: Industrialization of Biology: Making Nature Accessible and Affordable — ***Christine Santos***

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(753) Integrating Municipal and Industrial Waste into Biorefineries
Thursday, Nov 2, 3:15 PM
MCC, 101B

Emmanuel Revellame, Chair
Chenlin Li, Co-Chair

Sponsored by: Sustainable Biorefineries

3:15 Paper 753a: Production of Renewable Hydrogen from Wastewater Using Microbial Electrochemical Systems — ***Hong Liu***, *Luguang Wang, Stephanie Trujillo*

3:40 Paper 753b: Scale-Up and Process Intensification of Agricultural and Municipal Solid Waste Conversion Using Ionic Liquid–Based Process — ***Ning Sun***, *Ling Liang, Jipeng Yan, Qian He, Chenlin Li, Blake Simmons, Vicki S. Thompson, Seema Singh, Todd Pray*

4:05 Paper 753c: Map of Our Scrap: A GIS-Based Analysis on the Potential of Food Wastes for Bioenergy Production — ***Dhan Lord Fortela***, *Mark Zappi*

4:30 Paper 753d: Biochar from Excelsior Residues for Plantation Production of Hybrid Poplar — ***Catherine E. Brewer***, *Kwabena Sarpong, Andrea Salazar, Michael K. O'Neill, Delia Valles-Rosales, Fred Christiansen*

4:55 Paper 753e: Co-Pyrolysis of Plastics and Biomass Waste — *Nicholas R. Schwartz,* ***Michael J. Blaise***, *Alex D. Paulsen, Paul E. Yelvington*

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(754) Interfacial Phenomena in Ionic Liquids
Thursday, Nov 2, 3:15 PM
MCC, M100B

Paschalis Alexandridis, Chair
Lei Li, Co-Chair
Peng Jiang, Co-Chair

Sponsored by: Interfacial Phenomena

3:15 Paper 754a: Spreading of Nanoscale Droplets of Ionic Liquids on the Mica Surface — ***Lei Li***

3:30 Paper 754b: Long-Range Electrostatic Screening in Ionic Liquids — ***Matthew A. Gebbie***

3:45 Paper 754c: Mesopore Confinement Effects on Ionic Liquid Hydration — ***Yuxin He***, *Daudi Saang'onyo, Folami Ladipo, Barbara L. Knutson, Stephen E. Rankin*

4:00 Paper 754d: Water Sorption in Ionic Liquids Characterized Using a Dynamic Vapor Sorption Analyzer (IGASorp) and High-Pressure X-Ray Photoelectron Spectroscopy (APXPS) — ***M. Alejandra Rocha***, *Alicia Broderick, John T. Newberg, Mark B. Shiflett*

4:15 Paper 754e: Property Modeling of Ionic Liquids for Gas Separation Processes — ***Xinyan Liu***, *Xiaodong Liang, Xiangping Zhang, Suojiang Zhang, Rafiqul Gani*

4:30 Paper 754f: An Investigation of Cellulose Solubility in Ionic Liquids with Added Cosolvents — ***Brooks D. Rabideau***

4:45 Paper 754g: Effects of Ionic Liquids and Liposomes on Enzymatic Cellulose Hydrolysis Process — ***Kazuhiko Tanimura***, *Yoshiko Ooe, Keishi Suga, Yukihiro Okamoto, Makoto Yoshimoto, Hiroshi Umakoshi*

5:00 Paper 754h: Prediction of Energy Requirement for Recycling Ionic Liquids from Water After Cellulose Dissolution — ***Suojiang Zhang***, *Anne S. Meyer*

5:15 Paper 754i: Micellization of Poloxamer Block Copolymers in Ionic Liquids and Their Mixtures with Water — *Zhiqi He, Yingzhen Ma,* ***Paschalis Alexandridis***

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(755) Membrane-Based Organic Solvent Separations
Thursday, Nov 2, 3:15 PM
MCC, M100J

Andrew Livingston, Co-Chair
Ryan Lively, Co-Chair
Geoffrey M. Geise, Co-Chair

Sponsored by:
Membrane-Based Separations

3:15 Paper 755a: Polybenzimidazole-Based Membranes for Organic Solvent Nanofiltration (OSN) — ***Ruiyi Liu***, *Irina Valtcheva, Piers Gaffney, Patrizia Marchetti, Andrew Livingston*

3:33 Paper 755b: Organic Solvent Nanofiltration with Novel Perfluoropolymer Membranes and Other Novel Membrane Processes — *Prithish Basak, John Chau,* ***Kamalesh K. Sirkar***

3:51 Break

4:09 Paper 755d: Defect-Free PIM-1-Based Hollow Fiber Membranes — ***Melinda L. Jue***, *Ryan P. Lively*

4:27 Paper 755e: Extraction and Phase Separation of APIs in Low–Interfacial Tension Mixtures — ***Joseph Imbrogno***, *Luke Rogers, Dale Thomas, Klavs F. Jensen*

4:45 Paper 755f: Tunable Mesoporous Films from Graft Copolymers with Degradable Side Chains — ***Aaron M. Bush***, *Ruilan Guo, William A. Phillip*

5:03 Paper 755g: Effects of Pore Size in Polybenzimidazole Membranes on the Performance of Organic Solvent Nanofiltration — ***Jie Liu***, *Xian Kong, Jianwen Jiang*

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(756) Modeling, Control and Optimization of Energy Systems II
Thursday, Nov 2, 3:15 PM
MCC, 103D

Alexander W. Dowling, Chair
Edward P. Gatzke, Co-Chair

Sponsored by:
Systems and Process Control

3:15 Paper 756a: Enhanced Furnace Balancing Scheme via an Integrated Computational Fluid Dynamics/Data-Based Optimization Approach — ***Anh Tran***, *Marquis Crose, Andres Aguirre, Yangyao Ding, Helen Durand, Panagiotis D. Christofides*

3:34 Paper 756b: Stochastic Programming Approach vs. Estimator-Based Approach for Sensor Network Design for Maximizing Efficiency — ***Urmila M. Diwekar***, *Debangsu Bhattacharyya*

3:53 Paper 756c: Optimal Scheduling of a Microgrid on a Steam-Assisted Gravity Drainage (SAGD) Facility — ***Sagar N. Purkayastha***, *Yujun Chen, Jingyi Wang, David Layzell, Song Sit, Ian D. Gates, Milana Trifkovic*

4:12 Paper 756d: Design and Implementation of MPC Strategies for Supercritical Pulverized Coal-Fired Power Plant Cycling with Carbon Capture — ***Xin He***, *Fernando V. Lima*

4:31 Paper 756e: Fast Nonlinear Model Predictive Control Implementation with Open-Source Tools — ***David Thierry***, *Lorenz Biegler*

4:50 Paper 756f: Robust Stabilization of a Two-Stage Continuous Anaerobic Bioreactor — ***Zhaoyang Duan***, *Costas Kravaris*

5:09 Paper 756g: Receding-Horizon Optimal Operation and Control of a Solar-Thermal District Heating System — ***Xiaodong Xu***, *Yuan Yuan, Stevan Dubljevic*

5:28 Paper 756h: Control System Design for Small-Size-Isolated Concentrated Solar Power Generation Units — *Ashish Singh, Soorathep Kheawhom,* ***Nitin Kaistha***

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(757) MOFs, COFs, and Porous Polymer Materials II: Application
Thursday, Nov 2, 3:15 PM
MCC, 102C

Kumar Varoon Agrawal, Chair
Yongchul G. Chung, Co-Chair
Basudeb Saha, Co-Chair

Sponsored by: Inorganic Materials

3:15 Paper 757a: The Influence of Intrinsic Framework Flexibility on Adsorption in Nanoporous Materials — ***Matthew Witman***, *Sanliang Ling, Sudi Jawahery, Peter Boyd, Maciej Haranczyk, Ben Slater, Berend Smit*

3:34 Paper 757b: Towards a Generalized Understanding of Acid Gas Interactions with ZIF Materials — ***Souryadeep Bhattacharyya***, *Rebecca Han, David S. Sholl, Sankar Nair*

3:53 Paper 757c: Heat-Treatment of Defective UiO-66 from Modulated Synthesis: Adsorption and Stability Studies — *Yang Jiao,* ***Yang Liu***, *Krista S. Walton, David S. Sholl*

4:12 Paper 757d: Design of Stratified Hybrid Metal-Organic Frameworks for Chemical Detection and Destruction — ***Jonathan Ruffley***, *Tianyi Luo, Isabella Goodenough, Melissandre Richard, Eric Borguet, Nathaniel L. Rosi, J. Karl Johnson*

4:31 Paper 757e: Understanding Structure, Metal Distribution, and Water Adsorption in Mixed-Metal MOF-74 — ***Joshua D. Howe***, *Cody R. Morelock, Yang Jiao, Karena W. Chapman, Krista S. Walton, David S. Sholl*

4:50 Paper 757f: Extraction of Rare Earth Elements from Geothermal Brine Solution Using Magnetic Core-Shell Microspheres — ***Praveen K. Thallapally***, *Nune Satish, Jian Liu, B. Peter McGrail*

5:09 Paper 757g: Cycloaddition Reaction of Epoxides with CO_2 in a Copper Metal-Organic Framework: A Density Functional Theory Study — ***Xu Li***, *Jianwen Jiang*

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(758) Nanostructured Polymer Films
Thursday, Nov 2, 3:15 PM
MCC, 102D

Siamak Nejati, Chair
Amy M. Peterson, Co-Chair

Sponsored by: Polymers

3:15 Paper 758a: Nanostructured Materials for Separations Based on Reactive Block Polymers — ***Marc A. Hillmyer***

TECHNICAL SESSIONS 2017

3:45 Paper 758b: Block Copolymer–Derived Nanostructured Surfaces: Templating Confined Surface Reactions — ***Katherine P. Barteau***, *Katharine W. Oleske, Ulrich Wiesner, Lara A. Estroff*

4:00 Paper 758c: Nanostructure Formation on Collapse of Polyelectrolyte Brushes — ***Blair Kathryn Brettmann***

4:15 Paper 758d: iCVD Deposition and Integration of Poly-(1H,1H,2H,2H-Perfluorodecylacrylate) (PPFDA) Under High Loading of TiO_2 Nanoparticles — ***Zhengtao Chen***, *Kenneth K. S. Lau*

4:30 Paper 758e: Development of Resin-Containing Polymer Particles for Thermoset Powder Coatings — ***Guozhen Yang***, *Mengfei Huang, John Klier, Jessica D. Schiffman*

4:45 Paper 758f: Roll-to-Roll Micromolding of UV-Curable Thiol-Ene-Based Coatings — ***Yuyang Du***, *Alon McCormick, Lorraine F. Francis*

5:00 Paper 758g: Elastic Networks for Shape-Memory Contact Printing — ***Mitchell Anthamatten***

5:15 Paper 758h: Dynamics of Electric Double-Layer Formation and Dissipation in Polyethylene Oxide–$LiClO_4$ on Graphene Transistors — ***Susan Fullerton***, *Hua-Min Li, Ke Xu, Buchanan Bourdon, Hao Lu, Yu-Chuan Lin, Joshua Robinson, Alan Seabaugh*

5:30 Paper 758i: Redox-Active Organometallic Polymers for Small-Molecule Separations — ***Xiao Su***, *Timothy Jamison, T. Alan Hatton*

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(759) Novel Nanoparticles and Nanostructured Materials for Energy & Environmental Applications II
Thursday, Nov 2, 3:15 PM
MCC, 200H

Satish Nune, Chair
Alan W. Weimer, Co-Chair
Yangchuan Xing, Co-Chair

Sponsored by: Nanoparticles

3:15 Paper 759a: Silica Nanoparticles as Wettability Modifier and Mobility Control Agent in Enhanced Oil Recovery — ***Muhammad Shahzad Kamal***, *Farrukh Shehzad, Umer Mehmood*

3:35 Paper 759b: Hierarchical Porous Reduced Graphene Oxide as High-Performance Anode for Li-Ion Batteries — ***Huan Wang***, *Victoria Zane, Jingyi Xie, Xu Li, Placidus B. Amama*

3:55 Paper 759c: Synthesis, Fabrication, and Characterization of Thick Lithium-Ion Battery Electrodes (Invited) — ***Gary M. Koenig Jr.***, *J. Pierce Robinson, Adam Kern, Zhaoxiang Qi*

4:35 Paper 759d: Flower-Structured 1T Metallic-Phase MoS_2 as Electrode Materials for Solar Cells — ***Wei Wei***, *Yun Hang Hu*

4:55 Paper 759e: Scalable Self-Assembly of Nanoparticle Antireflection Coatings — ***Zhuxiao Gu***, *Peng Jiang*

5:15 Paper 759f: Hybrid Nanocoatings of Graphene-ZnO-Binder on Steel Surfaces to Reduce Friction and Wear Under High-Load Conditions — ***Vilas G. Pol***, *Arthur Dysart, Abdullah Alazemi, Farshid Sadeghi*

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(760) Novel Nanoparticles and Nanostructured Materials for Pharmaceuticals and Medical Applications
Thursday, Nov 2, 3:15 PM
MCC, 200J

Georgios A. Sotiriou, Chair
Alexandra Teleki, Co-Chair

Sponsored by: Nanoparticles

3:15 Paper 760a: Laying to Rest the Magnetically Dead Layer in Magnetic Nanoparticles — *Mythreyi Unni, Amanda Uhl, Shehaab Savliwala, Benjamin Savitzky, Rohan Dhavalikar, Nicolas Garraud, David P. Arnold, Lena Kourkoutis, Jennifer Andrew,* ***Carlos Rinaldi***

3:55 Paper 760b: Rapid and Facile PET Activation of Preformed Phthalocyanine Nanoparticles for Imaging Applications — ***Leon Z. Wang***, *Hoang D. Lu, Brian K. Wilson, Simon A. McManus, Prashanth Padakanti, Abass Alavi, Robert Mach, Robert K. Prud'homme*

4:15 Paper 760c: Modulating Antimicrobial Activity and Mammalian Cell Biocompatibility with Glycosylated Miktoarm Star Polymers — *Edgar H. H. Wong,* ***Zhangyong Si***, *Mary B. Chan-Park*

4:35 Paper 760d: Electrospinning Polymer Nanomedicines Extend Shelf-Life and Size Stability — ***Shani Levit***, *Ratib Stwodah, Christina Tang*

4:55 Paper 760e: In-Vitro Study of a Drug Delivery System Constituted by Levan and 5-Fluorouracil with Different Cancer Cell Lines with an Overexpression in GLUT5 — *Celia Nieto,* ***Antonio Tabernero***, *Álvaro González-Garcinuño, Miguel A. Galán, Eva M. Martín del Valle*

5:15 Paper 760f: The Influence of Fluid Dynamics on Nanomaterial Delivery Efficiency: Elucidating the Roles of Particle Size and Cell Model — ***Kristen K. Comfort***, *Katherine E. Burns, Robert F. Uhrig, Madison F. Bourbon*

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(761) Planning and Scheduling II
Thursday, Nov 2, 3:15 PM
MCC, 103E

Zukui Li, Chair
Jie Li, Co-Chair

Sponsored by:
Computers in Operations and Information Processing

3:15 Paper 761a: Strategic Planning of Oil Sands SAGD Drainage Area Development Under Uncertainty — *Farough Motamed Nasab, Hossein Shahandeh,* ***Zukui Li***

3:34 Paper 761b: A Multistage Stochastic Programming Approach to Long-Term Electricity Procurement for Large Industrial Consumers — ***Qi Zhang***, *Jose M. Pinto, Ignacio E. Grossmann*

3:53 Paper 761c: Multi-Stage Stochastic Programming Models for Pharmaceutical Clinical Trial Planning — ***Zuo Zeng***, *Selen Cremaschi*

4:12 Paper 761d: Two-Stage Stochastic Programming with Chance Constraints for Refinery Optimization — ***Yu Yang***

4:31 Paper 761e: An Improved Robust Optimization Approach for Scheduling Under Uncertainty — ***Utkarsh Shah***, *Yannis A. Guzman, Logan R. Matthews, Christodoulos A. Floudas*

4:50 Paper 761f: Adjustable Robust Optimization for Multi-Tasking Scheduling with Reprocessing of Imperfect Tasks — ***Nikolaos Lappas,*** *Luis A. Ricardez-Sandoval, Ricardo Fukasawa, Chrysanthos E. Gounaris*

5:09 Paper 761g: A Data-Driven Multistage Adaptive Robust Optimization Framework for Planning and Scheduling Under Uncertainty — ***Chao Ning***, *Fengqi You*

5:28 Paper 761h: Robust Refinery Planning Under Exogenous and Endogenous Uncertainty — ***Dimitrios Varvarezos***

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(762) Quality by Design in Drug Substance Process Development
Thursday, Nov 2, 3:15 PM
MCC, 101E

Yang Yang, Chair
Dominique Hebrault, Co-Chair

Sponsored by:
Pharmaceutical Discovery, Development and Manufacturing Forum

3:15 Paper 762a: Use of a Trickle-Bed Reactor to Improve the Commercial Feasibility of the Hydrogenation of a Nitro-Compound — ***Carla Luciani***, *Jonas Y. Buser, Michael Laurila, Richard Cope, Kevin P. Cole, Bradley M. Campbell, Justin Burt, Martin Johnson, Joseph Martinelli, David Mitchell*

3:40 Paper 762b: Use of Process Analytical Technology to Gain Mechanistic Insights into Spherical Agglomeration of Active Pharmaceutical Ingredients — ***Kanjakha Pal***, *Ramon Pena, Daniel Jarmer, Christopher L. Burcham, Zoltan K. Nagy*

4:05 Paper 762c: Process Dynamics of Continuous Cooling Crystallization of Carbamazepine in a Mixed-Suspension Mixed-Product Removal (MSMPR) System — ***David A. Acevedo***, *Xiaochuan Yang, Adil Mohammad, Naresh Pavurala, Wei-Lee Wu, Thomas O'Connor, Sau Lee, Patrick J. Faustino, Zoltan K. Nagy, Celia N. Cruz*

4:30 Paper 762d: Monte Carlo Stepwise Regression for More Accurate Selection of Critical Process Parameters During Process Characterization — ***Cary F. Opel***, *Cerintha J. Hui, Patrick Y. Yang, Daniel J. Tien*

4:55 Paper 762e: Delivering a Design Space for a Continuous Drug Substance Manufacturing Process Using Simulation — ***Neil Hodnett***

5:20 Paper 762f: Estimating NRTL-SAC Conceptual Segments of Molecules Using Sigma Profile — ***Yifan Hao,*** *M. R. Islam, Meng Wang, Chau-Chyun Chen*

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(763) Rare Earth Elements in Fossil Fuel–Derived Solids and Liquids
Thursday, Nov 2, 3:15 PM
MCC, 200C

Evan J. Granite, Chair
Tracy Bank, Co-Chair
Elliot Roth, Co-Chair
Mary Anne Alvin, Co-Chair

Sponsored by:
Advances in Fossil Energy R&D

3:15 Paper 763a: Leaching Rare Earth Elements (REEs) from Coal Ash by Mineral Acids — *Yan Luo,* ***Hanjing Tian***, *James C. Hower, Maohong Fan*

3:34 Paper 763b: Recovery of Rare Earth Elements from Coal Ash with a Recycling Acid Leach Process — ***Rick Peterson***

3:53 Paper 763c: Leaching Rare Earth Elements from Coal and Fly Ash Through Biochemical Processes — ***Yanna Liang***, *Stephen Park*

4:12 Paper 763d: Brief Overview of Rare Earth Research at NETL R&IC — ***Evan J. Granite***, *Elliot Roth, Tracy Bank, Ronghong Lin, Bret H. Howard, Yee Soong, McMahan L. Gray, Walter C. Wilfong, Ranjani V. Siriwardane*

4:31 Paper 763e: Extraction of Rare Earth Elements from Fly Ash Using NaOH Hydrothermal and Ultrasound Pretreatment — ***Elliot Roth***, *Megan Macala, Ronghong Lin, Tracy Bank, Bret H. Howard, Evan J. Granite*

4:50 Paper 763f: Recovery of Rare Earth Elements from North Dakota Lignite and Lignite-Related Feedstocks — ***Dan Laudal***, *Steve Benson*

5:09 Paper 763g: An Environmentally Friendly Approach to Recovery of Rare Earth Elements from Coal Production and Utilization Byproducts — ***Maohong Fan***

5:28 Paper 763h: Froth-Flotation Enrichment of Rare Earth Elements (REEs) from Different Feedstocks — ***Fan Shi***, *Yee Soong, McMahan L. Gray*

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(764) Rational Catalyst Design III: Metal Oxide and Compound Catalysis
Thursday, Nov 2, 3:15 PM
MCC, M100D

Siris Laursen, Chair
Meenesh R. Singh, Co-Chair
Matteo Cargnello, Co-Chair

Sponsored by:
Catalysis and Reaction Engineering Division

3:15 Paper 764a: Effects of Electrolyte Ions on Electrochemical CO_2 Reduction — ***Joaquin Resasco***, *Alexis T. Bell*

3:30 Paper 764b: Multifunctional Homogeneous-Heterogeneous Polymer Catalysts for the Synthesis of Hydroxymethylfurfural from Glucose — *Subhash Kalidindi, Anup Joshi, Deborah Dollard, Maria R. Coleman,* ***Ana C. Alba-Rubio***

3:45 Paper 764c: Nanobowls: A Platform for Selective Acid Catalysis on External Oxide Surfaces — ***Alexander Ardagh***, *Nicholas E. Thornburg, Zhenyu Bo, Scott Nauert, Justin M. Notestein*

4:00 Paper 764d: Controlled Tin Insertion into Zeolite Framework Vacancy Defects and Catalytic Consequences for Sugar Isomerization — ***Juan Carlos Vega-Vila***, *James W. Harris, Rajamani Gounder*

4:15 Paper 764e: Structure-Function Relationship Between Catalyst Hydrophobicity and Water Tolerance of Alkyl-Modified SBA-15-Supported Propylsulfonic Acid Catalysts — ***William Elliott***, *Robert M. Rioux*

4:30 Paper 764f: Promoted MoS_2 Edge Atoms for Highly Efficient CO_2 Conversion to Syngas — ***Pedram Abbasi***, *Mohammad Asadi, Cong Liu, Baharak Sayahpour, Larry A. Curtiss, Amin Salehi-Khojin*

4:45 Paper 764g: Framework-Topology-Dependent Catalytic Activity of Zirconium-Based, Porphyrinic Metal-Organic Frameworks — ***Diego Gomez Gualdron***, *Pravas Deria, Randall Q. Snurr, Joseph T. Hupp, Omar K. Farha*

5:00 Paper 764h: Constrained Geometry Single-Site Catalysts for Olefin Polymerization — ***Nikhil Prakash***

5:15 Paper 764i: Limitations of Top-Down Synthesis and Chloride-Based Bifunctional Polymer Solid-Acid Catalysts for Cellulose Hydrolysis — ***Maksim Tyufekchiev***, *Michael T. Timko, Marion Emmert, Sergio Granados-Focil, Pu Duan, Klaus Schmidt-Rohr*

5:30 Paper 764j: Advanced Catalyst for Energy Conversion and Storage Systems — ***Mohammad Asadi***

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(765) Semiconducting Quantum Dots II: Novel Syntheses and Devices
Thursday, Nov 2, 3:15 PM
MCC, 102B

Ayaskanta Sahu, Chair
Vincent C. Holmberg, Co-Chair

Sponsored by:
Electronics and Photonics

3:15 Paper 765a: Disorder, Nonequilibrium Transport, and the Origin of Deep Traps in Quantum Dot Solids — ***William A. Tisdale***

3:45 Paper 765b: On the Molecular Origin of Intra-Gap Emission from $CuInSe_{2-x}S_x$ Quantum Dots — ***Addis Fuhr***, *Nikolay Makarov, Hunter McDaniel, Hyeong Jin Yun, Hongbo Li, Anastassia Alexandrova, Phillippe Sautet, Victor I. Klimov*

4:01 Paper 765c: Accelerating Emission Dynamics in Perovskites Plasmonic Nanolasers — ***Sui Yang***, *Wei Bao, Xiaoze Liu, Xiang Zhang*

4:17 Break

4:27 Paper 765d: Synthesis and Characterization of Plasmon-Resonant Hollow Gold Nanoshells — ***Joesph A. Zasadzinski***, *JeongEun Shin*

4:57 Paper 765e: Solution-Based Synthesis of Cesium-Bismuth-Halide Perovskite Nanocrystals for Optoelectronic Applications — ***Rainie D. Nelson***, *Atefe Hadi, Alex Verburg, Matthew G. Panthani*

5:13 Paper 765f: Integrated Logic Gate Devices Fabricated Using Non-Toxic $CuInSe_2$ Quantum Dots — ***Hyeong Jin*** *Yun, Jaehoon Lim, Jeongkyun Roh, Darren Chi Jin Neo, Matt Law, Jeffrey M. Pietryga, Victor I. Klimov*

5:29 Paper 765g: Synthesis and Surface Functionalization of Group IV Quantum Dots — ***Yujie Wang***, *Michael Zembrzuski, Matthew G. Panthani*

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(766) Structure and Properties in Polymers
Thursday, Nov 2, 3:15 PM
MCC, 102E

Nese Orbey, Chair
Stephen M. Martin, Co-Chair

Sponsored by: Polymers

3:15 Paper 766a: Understanding Rate-Dependent Mechanical Properties of Supramolecular Hydrogels Through Real-Time SAXS Measurements During Stretching — ***Bryan D. Vogt***

3:45 Paper 766b: Microstructure and Mechano-Electrical Property of Ultra-Stretchable Iono-Elastomer via Small-Angle Scattering and Rheology — ***Ru Chen***, *Carlos R. López-Barrón, Norman J. Wagner*

4:00 Paper 766c: Toughening Isotactic Polypropylene with Block Copolymer Micelles — ***Jun Xu***, *Micah J. Howard, Frank S. Bates*

4:15 Paper 766d: The Importance of Crystalline Structure on the Tensile Properties of UHMWPE — ***Nicolas J. Alvarez***, *Christopher Henry, Giuseppe Palmese*

4:30 Paper 766e: Controlling Polymerization-Induced Phase Separation (PIPS) Using the Nonlinear Optical Properties of Light — ***Ian Hosein***, *Saeid Biria*

4:45 Paper 766f: Engineering Polymer Structure and Dispersity to Access Designer Materials with Exquisite Properties — ***Jimmy Lawrence***, *Eisuke Goto, Bernd Oschmann, Dongsub Kim, Jing Ming Ren, Craig J. Hawker*

5:00 Paper 766g: Thermal Bridges for Phonon Transport Through Short Polymer Chains in a Hydrogen-Bonded Polymer Composite — ***Nitin Mehra***, *Liwen Mu, Jiahua Zhu*

5:15 Paper 766h: The Effect of Pendant Alkyl Chain Length in Epoxy/Amine Thermosets: Material Properties and Water Barrier Properties — ***John Vergara***, *Joshua Sadler, John La Scala, Santosh Kumar Yadav, Giuseppe Palmese*

5:30 Paper 766i: Novel Chemistries for the Replacement of Methylenedianiline in Composites — ***Joseph F. Stanzione III***, *Owen M. Stecca, Alexander W. Bassett, Jayson D. Cosgrove, Kevin M. Schmalbach, Joshua M. Sadler, John J. La Scala*

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(767) Surface-Engineered and Responsive Membranes
Thursday, Nov 2, 3:15 PM
MCC, M100H

Haiqing Lin, Co-Chair
Dona Foster, Co-Chair
S. Ranil Wickramasinghe, Co-Chair

Sponsored by:
Membrane-Based Separations

3:15 Paper 767a: Application of a New Zwitterionic Membrane Surface Chemistry for Biofouling Control — ***Steven T. Weinman***, *Maria Bass, Viatcheslav Freger, Moshe Herzberg, Scott M. Husson*

3:33 Paper 767b: Facile Grafting of Zwitterions onto Membrane Surface to Enhance Antifouling Properties for Wastewater Reuse — ***Nima Shahkaramipour***, *Chong Cheng, Haiqing Lin*

3:51 Paper 767c: Peptoid-Grafted Hollow Fiber Membranes for Improved Biocompatibility — ***Neda Mahmoudi***, *Grant Harrison, Nawaf Alshammar, Jamie Hestekin, Shannon L. Servoss*

4:09 Paper 767d: Colloidal Foulant Behavior on Membrane Surfaces with Controlled Chemistry and Ordered Roughness — ***Anna Malakian***, *Steven Weinman, Sapna Sarupria, Scott M. Husson*

4:27 Paper 767e: Spatial Control of Grafted Polymers on Ultrafiltration Membrane: A New Horizon of AGET-ATRP — ***Ranil Wickramasinghe***, *Arijit Sengupta, Xianghong Qian*

4:45 Paper 767f: VO_x Surface Catalyst for Low-Cost, High-Performance Hydrogen-Permeable Vanadium Membranes — ***Thomas F. Fuerst***, *Sean T. B. Lundin, J. Douglas Way, Colin A. Wolden*

5:03 Paper 767g: The Role of PNIPAM in Degrading Chlorinated Contaminants in Water Using Iron/Palladium-Functionalized MF Membranes — ***Anthony Saad***, *Hongyi Wan, Dibakar Bhattacharyya*

(768) Advances in Algal Biorefineries
Friday, Nov 3, 8:00 AM
MCC, 101B

Robert Gardner, Chair
Sridhar Viamajala, Co-Chair

Sponsored by: Sustainable Biorefineries

8:00 Paper 768a: Hydrothermal Liquefaction of Microalgae and Co-Product Development — ***Kodanda Phani Raj Dandamudi***, *Tapaswy Muppaneni, Thinesh Selvaratnam, Melvin Mathew, Peter Lammers, Shuguang Deng*

8:25 Paper 768b: Multiphysics Simulation of Microalgae Growth in an Airlift Photobioreactor: Effect of Fluid Mixing and Shear Stress — ***Xi Gao***, *Bo Kong, R. Dennis Vigil*

8:50 Paper 768c: From Microalgal Starch to Biobutanol Production: A Combined Experimental and Computational Study — ***Gonzalo M. Figueroa-Torres***, *Jon Pittman, Constantinos Theodoropoulos*

9:15 Paper 768d: Techno-Economic Assessment of Microalgae Biorefineries for the Production of High-Value Chemicals — ***Melina Psycha***, *Antonis C. Kokossis*

9:40 Paper 768e: A Process Model for Converting Low-Lipid Microalgae into Biocrude Oil via Hydrothermal Liquefaction — ***Aersi Aierzhati***, *Yuanhui Zhang, Megan Swoboda, Peng Zhang, Wan-Ting Chen*

10:05 Paper 768f: Flocculation and Vacuum Filtration of Algal-Slurry Intermediates to Enable Parallel Algal Processing — ***Jonathan J. Stickel***, *Nicholas J. Nagle, Mason Minot, Nathan C. Crawford, Eric Knoshaug, Ali Mohagheghi, Tao Dong, Philip Pienkos*

(769) Bio-Based Polymers
Friday, Nov 3, 8:00 AM
MCC, 102A

Joseph F. Stanzione III, Chair
Bryan W. Boudouris, Co-Chair

Sponsored by: Polymers

8:00 Paper 769a: Strategic Assemblies of Wood-Derived Building Blocks for the Sustainable Redesign of BPA-Based Polymers — ***Joseph F. Stanzione III***, *John J. La Scala*

8:30 Paper 769b: Preparation and Characterization of Cardanol-Based Vinyl Ester Resins as Cross-Linker Units — ***Emre Kinaci***

8:45 Paper 769c: Ionic Liquids: Green Solvents for Dry Native Cellulose and Chitosan — ***Behzad Nazari***, *Nyalaliska Utomo, Sujyot Mony, Hyeonji Oh, Indira Saifuddin, Ralph H. Colby*

9:00 Paper 769d: Environmentally Friendly Flame Retardants Based on Adhesive Catecholamine — ***Hanim Kim***, *Joon Hee Cho, Kadhiravan Shanmuganathan, Amanda Jones, Sergei Nazarenko, Christopher J. Ellison*

9:15 Paper 769e: Soybean Oil–Based Thermoset Materials with High Biorenewable Content — ***Sung-Soo Kim***, *Dustin Janes, Kadhiravan Shanmuganathan, Daniel Y. Chou, Christopher J. Ellison*

9:30 Paper 769f: Carbon Fibers Derived from Fractionated-Solvated Lignin Precursor — ***Jing Jin***, *Adam S. Klett, Junhuan Ding, Mark C. Thies, Amod A. Ogale*

9:45 Paper 769g: Self-Assembly of Coil-Hyperbranched Poly(styrene-block-acrylated epoxidized soybean oil) Block Copolymers — ***Fang-Yi Lin***, *Austin D. Hohmann, Nacu Hernandez, Eric W. Cochran*

10:00 Paper 769h: Physicochemical Properties of Polylactide/Delta-Valerolactone/Organosolv Lignin Atactic Terpolymers — ***Stephanie Harris***, *Ulrike Tschirner, Adam Gillespie, Madeleine Seeger*

10:15 Paper 769i: Oil Field Chemicals from Macromolecular Renewable Resources: Date Pit as a Case Study for Drilling Fluid Additive — ***Jimoh K. Adewole***, *Musa O. Najimu*

(770) Biomaterials for In-Vitro Tissue Models and Improved Therapeutic Strategies
Friday, Nov 3, 8:00 AM
MCC, 102E

Shreyas Rao, Chair
Kyle Lampe, Co-Chair

Sponsored by: Biomaterials

8:00 Paper 770a: Designing Synthetic Extracellular Matrices for the Creation of Controlled Culture Systems in the Study of Disease — ***April M. Kloxin***

8:36 Paper 770b: The Influence of Matrix Stiffness on the Behavior of Brain Metastatic Breast Cancer Cells — ***Akshay Narkhede***, *Shreyas Rao*

8:54 Paper 770c: The Combined Effect of Matrix Microenvironment and Hypoxia on the Activity of Glioblastoma Stem Cells — ***Jee-Wei Emily Chen***, *Jann N. Sarkaria, Brendan A. Harley*

9:12 Paper 770d: Glioblastoma/Astrocyte Co-Culture on Polyelectrolyte Multilayer Films: A Template for Studying the Role of Astrocytes in Glioblastoma Progression — ***Kimberly M. Stanke***, *Christina Wilson, Erin Eickman, Oleh Khalimonchuk, Srivatsan Kidambi*

9:30 Paper 770e: Three-Dimensional Tissues Using Human Pluripotent Stem Cell Spheroids as Biofabrication Building Blocks — ***Qiang Li***, *Haishuang Lin, Yuguo Lei*

9:48 Paper 770f: Dynamic Culture of Trabecular Meshwork Cells in 3D Biomimetic Scaffolds — ***Matthew Osmond***, *Mina Pantcheva, Melissa Krebs*

10:06 Paper 770g: Cellular Hitchhiking on Microparticles to Alleviate Skin Injury — ***Daniel Smith***, *Chase Herman, Sutapa Barua*

(771) Biomimetic Materials II: Applications
Friday, Nov 3, 8:00 AM
MCC, 102F

Zhiqiang Cao, Chair
Adrianne M. Rosales, Co-Chair
Nitin Agrawal, Co-Chair
Wei Li, Co-Chair

Sponsored by: Biomaterials

8:00 Paper 771a: Sugar-Coating the Answers to Virus Binding: Glycocalyx-Mimetic Interfaces — ***Ramya Kumar***, *Domenic Kratzer, Kenneth Cheng, Irina Kopyeva, Joerg Lahann*

8:18 Paper 771b: Glucose-Derived Cationic Block Poly(beta-peptides) Reverse Intrinsic Antibiotic Resistance in Gram-Negative Pathogens — ***Zhangyong Si***, *Hui Wen Lim, Damien Keogh, Moon Tay Yue Feng, Jo Thy Lachumy Subramanion, Yahua Chen, Guillermo C. Bazan, Everett Peter Greenberg, Yunn-Hwen Gan, Kevin Pethe, Mary B. Chan-Park*

8:36 Paper 771c: Mechanism Study of Selective Killing of Cationic Peptidopolysaccharide Nanoparticles with In-Vitro and In-Vivo Efficacy Against Multi-Drug-Resistant Bacteria — ***Mary Chan***, *Hou Zheng, Yogesh Vikhe*

8:54 Paper 771d: Tether-Supported Biomembranes with Phase Composition and Orientation Control for Biomaterial Ligand Displays and Membrane Protein Assays — ***William Houlihan***, *Yueming Li, Lane Gilchrist*

9:12 Paper 771e: Understanding the Interaction of the Polysaccharide, Chitosan, with a Novel Cuticular Protein, CPR 27, Using Quartz Crystal Microbalance with Dissipation — ***Aishik Chakraborty***, *Ellie K. Onstott, Neal T. Dittmer, Michael R. Kanost, Stevin H. Gehrke, Prajnaparamita Dhar*

9:30 Paper 771f: Probing Phase Transitions in Dynamic Biopolymer Complexation — ***Amanda B. Marciel***, *Handan Acar, Matthew V. Tirrell*

9:48 Paper 771g: Photo-Induced Pinocytosis in Synthetic Liposomes — ***Danielle Konetski***, *Dawei Zhang, Christopher Bowman*

10:06 Paper 771h: Protein Protection and Purification Through Virus-Like Particle Encapsidation: A Rapid 2-Step Cell-Free Protein Synthesis Approach — ***Bradley C. Bundy***, *Seung Ook Yang*

(772) Engineering Geologic Carbon Dioxide Storage Systems
Friday, Nov 3, 8:00 AM
MCC, 101A

Kanwal Mahajan, Chair
Rameshwar Srivastava, Co-Chair

Sponsored by: Advances in Fossil Energy R&D

8:00 Paper 772a: Geologic Storage of Carbon Dioxide in the Central Plains of North America — *David Nakles, Wesley D. Peck, Neil Wildgust, John A. Hamling,* ***Charles D. Gorecki***, *Edward N. Steadman, John A. Harju*

8:22 Paper 772b: Defining CO_2 Storage Options in the Upper Ohio River Valley: Advanced Characterization of Geologic Reservoirs and Caprocks — ***Caitlin McNeil***, *Neeraj Gupta, Mark Kelley, Autumn Haagsma, Isis Fukai, Amber Conner, Joel Main, Priya Ravi Ganesh, Samin Raziperchikolaee, Jared Hawkins*

8:44 Paper 772c: Impact of Brine/CO_2 Exposure on the Transport and Mechanical Properties of Mt. Simon Rock Samples — ***Zhuofan Shi***, *Lin Sun, Kristian Jessen, Theodore Tsotsis*

9:06 Paper 772d: Assignment and Calibration of Relative Permeability by Hydrostratigraphic Units: A Novel Approach for Multiphase Flow Analyses — Case Study Example: CO_2-EOR Operations at the Farnsworth Unit, Texas — ***Nathan Moodie***, *William Ampomah, Wei Jia, Brian McPherson*

9:28 Paper 772e: Development and Evaluation of an Iridium Oxide—Based Chemical Sensor for Downhole CO_2 Monitoring — ***Sai Wang***, *Kegang Ling, Hongsheng Wang, Ning Liu*

9:50 Paper 772f: Monitoring Carbon Sequestration Using Charged Wellbore Controlled Source Electromagnetics and Integrated Reservoir Models — ***Trevor Irons***, *Jiajia Sun, Nathan Moodie, Rich Krahenbuhl, Yaoguo Li, Brian McPherson, William Ampomah*

10:10 Paper 772g: Development of LIBS Sensor for Sub-Surface CO_2 Leak Detection in Carbon Sequestration — ***Jinesh Jain***, *Christian Goueguel, Dustin McIntyre*

(773) Molecular Simulation of Protein Adsorption and Molecular Recognition Processes
Friday, Nov 3, 8:00 AM
MCC, 103A

Heather Mayes, Chair
Liqun Zhang, Co-Chair
Jeremy C. Palmer, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

8:00 Paper 773a: Deep Cavity Cavitand/Alkane Assembly State Switching Between Monomeric and Dimeric Host–Guest Assemblies Driven by Guest Packing — ***Du Tang***, *J. Wesley Barnett, Bruce C. Gibb, Henry S. Ashbaugh*

8:15 Paper 773b: Elucidating Protein (Folding) Kinetics near Organic Surfaces as a Function of Surface Hydrophobicity — ***Elif Irem Senyurt***, *Gül H. Zerze, Jeetain Mittal*

8:30 Paper 773c: Serum Albumin Interactions with Doxorubicin-Loaded Graphene Oxide in an Aqueous Environment with Blood pH Level: A Molecular Dynamics Simulation Study — ***Mina Mahdavi***, *Sasan Nouranian, Ali Fattahi*

8:45 Paper 773d: Elucidating the Interaction Mechanisms of Thermo-Responsive Ligand with Proteins — ***Xiaoquan Sun***, *Xianghong Qian*

9:00 Paper 773e: Study of Interaction and Transpassing of Human Beta Defensin-3 with POPG and POPS Membrane — ***Rabeta Yeasmin***, *Liqun Zhang*

9:15 Paper 773f: Free-Energy Calculation for Microcin J25 Variants Binding to the FhuA Receptor and to RNA Polymerase — ***Pin-Kuang Lai***, *Yiannis Kaznessis*

9:30 Paper 773g: Predicting the Dimer Structure of Defensins Using a Combined Simulation Strategy — ***Liqun Zhang***, *Zhiming Feng, Aaron Weinberg*

9:45 Paper 773h: Full-Atom Molecular Simulations of Lysozyme Confined in Realistic Silica Mesopores: Insights in Conformation and Accessibility of Active Sites — ***Katarzyna Maksimiak***, *Richard Catlow, Alberto Striolo, Marc-Olivier Coppens*

10:00 Paper 773i: Aggregation and Self-Assembly of Biomimetic Polymers at Interfaces — ***Arushi Prakash***, *Christopher J. Mundy, Jim Pfaendtner*

(774) Multifunctional Composites
Monday, Oct 30, 12:30 PM
MCC, 211D

Zhengtang Luo, Chair
Luyi Sun, Co-Chair
Nurxat Nuraje, Co-Chair

Sponsored by: Composites

12:30 Paper 774a: Multifunctional Polymer Nanocomposites — ***Zhanhu Guo***, *Jiang Guo, Alexandra Galaska, Huige Wei, Suying Wei, Bin Qiu, Dawei Jiang, Hongbo Gu, Jiahua Zhu*

12:45 Paper 774b: Transparent Copper-Silica Nanoparticle-Chitosan Nanocomposite Coatings with Long-Term Antibacterial Efficacy — ***Debirupa Mitra***, *Min Li, En-Tang Kang, Koon Gee Neoh*

1:00 Paper 774c: Bio-Inspired Design of Stimuli Responsive Materials Based on a Bilayer Structure — *Songshan Zeng, Rui Li, Dianyun Zhang, Wenhan Huang, Zhaofeng Wang, Stephan Freire, Andrew Smith, Emily Huang, Helen Nguon, Xiaoyuan Yu,* ***Luyi Sun***

1:15 Paper 774d: Biomimetic Nanocoatings with Exceptional Mechanical, Barrier, and Flame Retardant Properties from Large Scale One-Step Co-Assembly — *Fuchuan Ding, Jingjing Liu, Songshan Zeng, Yan Xia, Kacie M. Wells, Mu-Ping Nieh,* ***Luyi Sun***

1:30 Paper 774e: Bioinspired Composite Materials with Stimuli-Responsive Color Changing Ability — *Golnaz Isapour,* ***Marco Lattuada***

1:45 Paper 774f: Investigation of Carbon Nanotubes & Cellulose Nanocrystals Composite for Potential Use in Microelectromechanical Systems — ***Mingzhe Jiang***, *Christopher L. Kitchens, Robert Seney, Bayliss Charles*

2:00 Paper 774g: Few Layers $MoSe_2$ Incorporated with Nitrogen Doped Graphene Sheet for High Performance Lithium Sulfur Batteries — ***Hoi Lun Wong, Zhengtang Luo***

2:15 Paper 774h: Dual-Responsive Plasmonic Behavior of Gold Nanorods@PANI Core/Shell Nanostructures for Real-Time Control — ***Ju-Won Jeon***, *Jing Zhou, Jeffrey Geldmeier, James Ponder, Mahmoud A. Mahmoud, Mostafa El-Sayed, John Reynolds, Vladimir V. Tsukruk*

2:30 Paper 118b: Microwave-Induced Heating of Carbon Nanotubes Localized at 3D-Printed Thermoplastic Interfaces — *Charles Sweeney, Mohammad Saed,* ***Micah Green***

(775) Nanostructured/Thin-Film Photovoltaics
Friday, Nov 3, 8:00 AM
MCC, 102B

Joshua Choi, Chair
Andrej Lenert, Co-Chair

Sponsored by: Electronics and Photonics

8:00 Paper 775a: Measurement and Modeling of Carrier Dynamics in Photovoltaic CZTSe — *Siming Li, Michael L. Lloyd, Brian E. McCandless,* ***Jason B. Baxter***

8:18 Paper 775b: Impact of the Active-Layer Morphology on Bimolecular Recombination Dynamics in Organic Solar Cells — *Veaceslav Coropceanu, Jean-Luc Brédas,* ***Shafigh Mehraeen***

8:36 Paper 775c: Atomistic Origin of the Concentration Dependence of Si Dopant Mobility in III-V Semiconductor Alloys — ***Mardochee Reveil***, *Paulette Clancy*

8:54 Paper 775d: Characterizing Defects in Photovoltaic Semiconductors with Optical Spectroscopy — ***Charles J. Hages***, *Thomas Unold*

9:12 Paper 775e: CIGS Nanocrystal Solar Cells on Plastics and Paper — *Vikas Reddy Voggu, Sam Morehead, Brian A. Korgel,* ***Taylor B. Harvey***

9:30 Paper 775f: Solution-Processed Thin-Film Photovoltaics Using Amine-Thiol Chemistry — ***Swapnil Dattatray Deshmukh***, *Xin Zhao, Ruihong Zhang, Caleb Miskin, David Rokke, Carol Handwerker, Rakesh Agrawal*

9:48 Paper 775g: Photonic Mirrors for Enhanced Optical Transport in Luminescent Solar Concentrators — ***Ryan Connell***, *Mayank Puri, Vivian E. Ferry*

10:06 Paper 775h: Dopant-Mediated Assembly of Nanorods into Atomically Coupled 2D Sheets in Solution — ***Ajay Singh***, *Delia J. Milliron*

(776) Particle Engineering as Applied to Pharmaceutical Formulations
Friday, Nov 3, 8:00 AM
MCC, 101D

Steven J. Brenek, Chair
Brendon G. Ricart, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

8:00 Paper 776a: Long-Term Coating Predictions for a Wurster Fluidized-Bed Coater Using a Combined CFD-DEM and Markov-Chain Monte Carlo Approach — ***Peter Toson***, *Peter Böhling, Maximilian Besenhard, Dalibor Jajcevic, Alan Carmody, Conrad Davies, Pankaj Doshi, Mary T. am Ende, Avik Sarkar*

8:23 Paper 776b: Microfluidization as an Enabling Technology for Solubility Enhancement — ***Íris Duarte***, *Clara Sá Couto, Tiago Porfírio, João Vicente, Márcio Temtem*

8:46 Paper 776c: Droplet-Templated Anti-Solvent Spherical Crystallization of Hydrophilic and Hydrophobic Drugs with an In-Situ-Formed Binder — ***Tonghan Gu***, *Saif A. Khan, T. Alan Hatton*

9:09 Paper 776d: Study and Control of the Flow Properties of Ibuprofen from Crystallization — ***Yunliang He***, *Yuan Gao, Brian Glennon, Anne-Marie Healy, Zelalem Worku*

9:32 Paper 776e: Formation and Dissolution Characteristics of Paracetamol Granules — ***Adetutu Martins***, *Adewale Lawal, Sheena Reeves*

9:55 Paper 776f: Size Reduction Through Flash Nanoprecipitation to Improve Solubility, Dissolution, and Bioavailability of Clofazimine — ***Yingyue Zhang***, *Jie Feng, Simon A. McManus, Hoang D. Lu, Kurt D. Ristroph, Robert K. Prud'homme*

10:18 Paper 776g: Discrete Element Modeling to Predict Pharmaceutical Powder Flow at Different Humidity Conditions — ***Raj Mukherjee***, *Sayantan Chattoraj, Chen Mao, Bodhisattwa Chaudhuri*

(777) Polymers in Additive Manufacturing
Friday, Nov 3, 8:00 AM
MCC, 102D

Amy M. Peterson, Chair
Blake Johnson, Co-Chair

Sponsored by: Polymers

8:00 Paper 777a: Tailored Polymers for Structural Application in Large-Scale Extrusion Systems — ***Blake Marshall***

8:30 Paper 777b: Modeling Flow Phenomena in Fused Filament Fabrication Geometry — ***Eric L. Gilmer***, *Darren Miller, Jacob Fallon, Camden Chatham, Callie Zawaski, Allison M. Pekkanen, Timothy E. Long, Christopher B. Williams, Michael J. Bortner*

8:45 Paper 777c: Influence of Processing on Additively Manufactured Mechanically Adaptive Cellulose Nanocrystal Polymer Composites — ***Jacob Fallon***, *Michael J. Bortner, Earl J. Foster, Cara Herwig, Ben Kolb*

9:00 Paper 777d: 3D-Printed Shape Memory Objects Based on Olefin Ionomer of Zinc-Neutralized Poly(ethylene-co-methacrylic acid) — ***Bryan D. Vogt***

9:15 Paper 777e: Three-Dimensional Printing by Multiphase Silicone/Water Capillary Inks — *Sangchul Roh, Dishit Parekh, Bhuvnesh Bharti, Simeon Stoyanov,* ***Orlin D. Velev***

9:30 Paper 777f: 3D Printing of Polymer-Bonded Magnets Using a Combination of Extrusion Direct-Write and Stereolithography Methods — ***Alan Shen****, Anson W. K. Ma, Sameh Dardona*

9:45 Paper 777g: PDMS-Based Ink Development for 3D Printing Applications — ***Kwan-Soo Lee****, Joseph H. Dumont, Andrew M. Schmalzer, ChiHoon Park, Andrea Labouriau*

10:00 Paper 777h: 3D-Printed Active Microfluidic Elements for Portable Bioanalysis Assays — ***Duanduan Han****, Victor M. Ugaz*

10:15 Paper 777i: 3D-Printed Polymer-Based Bio-Inspired Neural Systems — ***Blake Johnson***

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(778) Quality by Design in Drug Product Formulation, Design, and Process Development
Friday, Nov 3, 8:00 AM
MCC, 101E

Zhigang Sun, Chair
Ingmar Nopens, Co-Chair

Sponsored by:
Pharmaceutical Discovery, Development and Manufacturing Forum

8:00 Paper 778a: Formulation Strategies for Solid Dispersions Containing Tablets — ***Slavomira Doktorovova****, Evelyn Voney, João Henriques*

8:25 Paper 778b: Modeling the Effects of Material Properties on Tablet Compaction: A Case Study for Development — ***M. Sebastian Escotet-Espinoza****, Shishir Vadodaria, Fernando J. Muzzio, Marianthi Ierapetritou*

8:50 Paper 778c: Quality by Design Approaches for Dry Powder Inhalation Products: A Regulatory Perspective —***ChiaoChun J. Wang****,* ***Yong Hu****, Zhigang Sun*

9:15 Paper 778d: Effect of Bulk Properties of the Tracer on the Measurement of Residence Time Distributions in Continuous Powder-Based Unit Operations — *Sarang Oka, M. Sebastian Escotet-Espinoza, Andrés D. Román-Ospino, Yifan Wang, Marianthi Ierapetritou,* ***Fernando J. Muzzio***

9:40 Paper 778e: Assessing Suspension Homogeneity Using CFD-DEM for Enhanced Content Uniformity of Spray-Dried Intermediates — ***Nuno Enes****, Luís Eça, José Pereira, Ines Matos, Pedro Valente*

10:05 Paper 778f: Advanced Model Predictive Control of Powder Level in Continuous Pharmaceutical Manufacturing Pilot Plant — ***Ravendra Singh****, Fernando J. Muzzio, Marianthi Ierapetritou, Rohit Ramachandran*

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(779) Reactor Engineering for Biomass Feedstocks
Friday, Nov 3, 8:00 AM
MCC, 101C

Yukihiko Matsumura, Chair
Quang Nguyen, Co-Chair

Sponsored by: Sustainable Biorefineries

8:00 Paper 779a: Study on Mechanism of Clinker Formation in Bamboo Combustion Process — ***Shohei Okubo****, Ken-ichiro Tanoue, Tatsuo Nishimura, Miki Taniguchi, Ken-ichi Sasauchi*

8:25 Paper 779b: Modeling Pyrolysis-Induced Microstructural Changes in Biomass: A Cellular Automata Approach — ***Joseph Biernacki****, Michael Adenson*

8:50 Paper 779c: Shrinking and Heat and Mass Transfer During Pyrolysis of Woody Biomass — ***Ken-ichiro Tanoue****, Tatsuo Nishimura, Yoshimitsu Uemura, Miki Taniguchi, Ken-ichi Sasauchi*

9:15 Paper 779d: Plasma Gasification of Wood Pellets Using a Laboratory-Scale Plasma Reactor to Produce Synthesis Gas: Effect of Increasing Temperature and Addition of Oxygen to the Process — ***Ralph Muvhiiwa****, Diane Hildebrandt, Baraka Celestin Sempuga, Xiaojun Lu*

9:40 Paper 779e: Multistage Fluidized-Bed Reactor for Gasification — ***Sireesha Aluri****, Pradeep K. Agrawal, Carsten Sievers, John D. Muzzy, Derrick W. Flick, Ildar Musin*

10:05 Paper 779f: Overall View of Lignocellulosic Biomass Decomposition in Supercritical Water — ***Yukihiko Matsumura****, Nattacha Paksung, Rahmat I. Mainil*

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(780) Poster Session: Symposium on Solar Power and Chemical Systems in Honor of Prof. Edward A. Fletcher
Monday, Oct 30, 3:15 PM
MCC, Exhibit Hall B

Wojciech Lipinski, Chair
Nick AuYeung, Co-Chair
Alexandre Yokochi, Co-Chair

Sponsored by:
Symposium on Solar Power and Chemical Systems in Honor of Prof. Edward A. Fletcher

Paper 780a: Assessing the Thermodynamic Viability of Mixed Metal Oxides for Solar Thermochemical Water Splitting — ***Samantha L. Millican****, Kevin Sun, Iryna Androshchuk, Alan W. Weimer, Charles B. Musgrave*

Paper 780b: Thermodynamic Characterization of Charge-Compensating Double-Doped Ceria for Improved Redox Performance of Solar Thermochemical H_2O/CO_2 Splitting Cycles — ***Marie Hoes****, Christopher L. Muhich, Aldo Steinfeld*

Paper 780c: Solar Thermochemical Methane Reforming Using Metal Oxide Oxygen Exchange Materials — ***Georgina Ims****, Diana Tulip, Peter Kreider, Wojciech Lipinski*

Paper 780d: Oxide-Independent Thermodynamics of Solar Chemical-Looping Reforming for Producing Synthesis Gas and Hydrogen — ***Peter Krenzke****, Jane H. Davidson*

Paper 780e: Experimental Investigation of Carbon Dioxide Capture and High-Temperature Thermal Energy Storage via Metal Oxide Chemical Looping in a Prototype Reactor for Solar Thermochemical Metal Oxide Looping — ***José I. Zapata Fuentealba****, Lindsey Yue, Wojciech Lipinski*

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(781) Smart Manufacturing – the Clean Energy Smart Manufacturing Innovation Institute
Tuesday, Oct 31, 3:15 PM
MCC, 101A

Scott McWhorter, Chair
Yarom Polsky, Co-Chair
Phillip R. Westmoreland, Co-Chair

Sponsored by:
Next-Gen Manufacturing

3:15 Introductory Remarks

3:20 Paper 781a: Key Note Presentation Overviewing the Clean Energy Smart Manufacturing Innovation Institute — ***Jim Wetzel***

4:00 Paper 781b: Real-Time Adaptive Control of Carbon Fiber Production — ***Yarom Polsky***

4:15 Paper 781c: Smart and Advanced Manufacturing Innovation in DOE — ***Sudarsan Rachuri***

4:30 Paper 781d: Technology and Vision of Smart Manufacturing — ***Jim Davis***

4:45 Paper 781e: Panel Discussion on the Impacts of Smart

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(782) Finding a Healthy Work-Life Balance amid High Stress
Tuesday, Oct 31, 12:30 PM
MCC, 102C

Martin Siron, Chair

Sponsored by:
Young Professionals Committee (YPC)

DID YOU KNOW?

Minneapolis native Dr. C. Walton Lillehei was the first surgeon to perform a successful open-heart surgery at the University of Minnesota in 1953.

AIChE Events Calendar

PROFESSIONAL DEVELOPMENT

AIChE® is the global home of over 53,000 chemical engineers in more than 110 countries, with a breadth of resources, education offerings, networking and presentation opportunities. Members access technical information, find learning opportunities from recognized authorities, and always receive the lowest registration rates for conferences. Move forward professionally with AIChE and enrich the world we live in.

AIChE Conferences & Events

NOV. 14 – 15, 2017
2017 European Conference on Process Safety and Big Data (Co-sponsored by CCPS and EPSC)
DECHEMA House • Frankfurt am Main, Germany

DEC. 3, 2017
2017 Rock Stars of Regenerative Engineering
Beckman Center • Irvine, CA

DEC. 4 – 6, 2017
International Conference on CRISPR Technologies (Sponsored by SBE)
Raleigh Convention Center • Raleigh, NC

DEC. 13 – 15, 2017
International Conference on Epigenetics and Bioengineering (Sponsored by SBE)
The Palms Hotel and Spa • Miami, FL

JAN. 8 – 10, 2018
8th International Conference on Biomolecular Engineering (ICBE Asia 2018; Sponsored by SBE)
Grand Hyatt Singapore • Singapore

MAR. 11 – 14, 2018
International Conference on Accelerated Carbonation for Environmental and Material Engineering (ACEME)
Newcastle City Hall • Newcastle, New South Wales, Australia

APR. 22 – 26, 2018
2018 AIChE Spring Meeting and 14th Global Congress on Process Safety
Orlando World Center Marriott • Orlando, FL
8th World Congress on Particle Technology
Orlando World Center Marriott • Orlando, FL

JUN. 3 – 7, 2018
2018 Synthetic Biology: Engineering, Evolution & Design (SEED)
Scottsdale Camelback Resort • Scottsdale, AZ

JUN. 5 – 7, 2018
2018 Process Development Symposium
Hyatt Lodge at Hamburger University • Oak Brook, IL

JUN. 24 – 28, 2018
Metabolic Engineering 12
The Westin Grand Munich • Munich, Germany

SEPT. 16 – 20, 2018
63rd Annual Safety in Ammonia Plants and Related Facilities Symposium
Sheraton Centre Toronto Hotel • Toronto, ON, Canada

OCT. 4 – 5, 2018
10th AIChE Southwest Process Technology Conference
Moody Gardens Hotel and Convention Center
Galveston, TX

OCT. 28 – NOV. 2, 2018
2018 AIChE Annual Meeting
David L. Lawrence Convention Center • Pittsburgh, PA

AIChE Academy

NOV. 13 – 14, 2017
Crystallization Operations
Public Course • Houston, TX

NOV. 16, 2017
Use Your Data to Its Full Potential to Prevent Outages
Sponsored Webinar • LIVE Thursday, 2:00 PM-3:00 PM EST

DEC. 4 – 6, 2017
CCPS' HAZOP Studies and Other PHA Techniques for Process Safety and Risk Management
Public Course • Houston, TX

DEC. 4 – 8, 2017
CCPS' HAZOP Studies/Advanced PHA Concepts Combo Course
Public Course • Houston, TX

DEC. 5 – 6, 2017
Flow of Solids in Bins, Hoppers, Chutes and Feeders
Public Course • Houston, TX

DEC. 5 – 7, 2017
Essentials of Chemical Engineering for Non-Chemical Engineers
Public Course • Houston, TX

DEC. 7, 2017
Pneumatic Conveying of Bulk Solids
Public Course • Houston, TX

DEC. 7 – 8, 2017
CCPS' Advanced Concepts for Process Hazard Analysis
Public Course • Houston, TX

DEC. 11 – 14, 2017
CCPS' Process Safety Boot Camp
Public Course • Houston, TX

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institute for sustainability — An AIChE Technological Community
imes — International Metabolic Engineering Society
International Society for Water Solutions — An AIChE Technological Community
Society for Biological Engineering — An AIChE Technological Community
RAPID — Transforming Process Industries

For information and registration details, visit www.aiche.org

2017 ANNUAL MEETING SESSION PARTICIPANTS

Please note: Bold-faced numbers alone denote either a chair or co-chair.
Bold-faced numbers with letters denote speakers.

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SESSION PARTICIPANTS

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2017 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 AIChE Staff members is required by AIChE. The training program is coordinated by AIChE's Human Resources Department. For more information on this topic, please contact **humanresources@aiche.org**.

AIChE® VOLUNTEER + MEETING ATTENDEE CONDUCT GUIDELINES

AIChE's volunteers are the core of the Institute and make all of its programs, conferences and educational efforts possible. These offerings provide excellent opportunities for AIChE members and meeting attendees to gain greater technical expertise, grow their networks, and enhance their careers. AIChE events provide engineers, scientists, and students a platform to present, discuss, publish and exhibit their discoveries and technical advances.

At all times, volunteers and meeting attendees should act in accordance with AIChE's Code of Ethics, upholding and advancing the integrity, honor and dignity of the chemical engineering profession. AIChE's Board of Directors has developed these guidelines to foster a positive environment of trust, respect, open communications, and ethical behavior. These guidelines apply to meetings, conferences, workshops, courses and other events organized by AIChE or any of its entities and also to volunteers who conduct other business and affairs on behalf of AIChE.

SPECIFICALLY:

1. Volunteers and meeting attendees should understand and support AIChE's Code of Ethics.
2. Volunteers and meeting attendees should contribute to a collegial, inclusive, positive and respectful environment for fellow volunteers and attendees, and other stakeholders, including AIChE staff.
3. Volunteers and meeting attendees should avoid making inappropriate statements or taking inappropriate action based on race, gender, age, religion, ethnicity, nationality, sexual orientation, gender expression, gender identity, marital status, political affiliation, presence of disabilities, or educational background. We should show consistent respect for colleagues, regardless of discipline, employment status, and organizations for which they work, whether industry, academia, or government.
4. Disruptive, harassing or other inappropriate statements or behavior toward other volunteers, members, and other stakeholders, including AIChE staff, is unacceptable.
5. Volunteers and meeting attendees should obey all applicable laws and regulations of the relevant governmental authorities while volunteering or attending meetings. Volunteers and meeting attendees taking part in any AIChE event, including the Chem-E-Car Competition®, should also comply with all applicable safety guidelines.

Any violations of the foregoing should be reported to the President or the Executive Director of the Institute.

NOTES


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