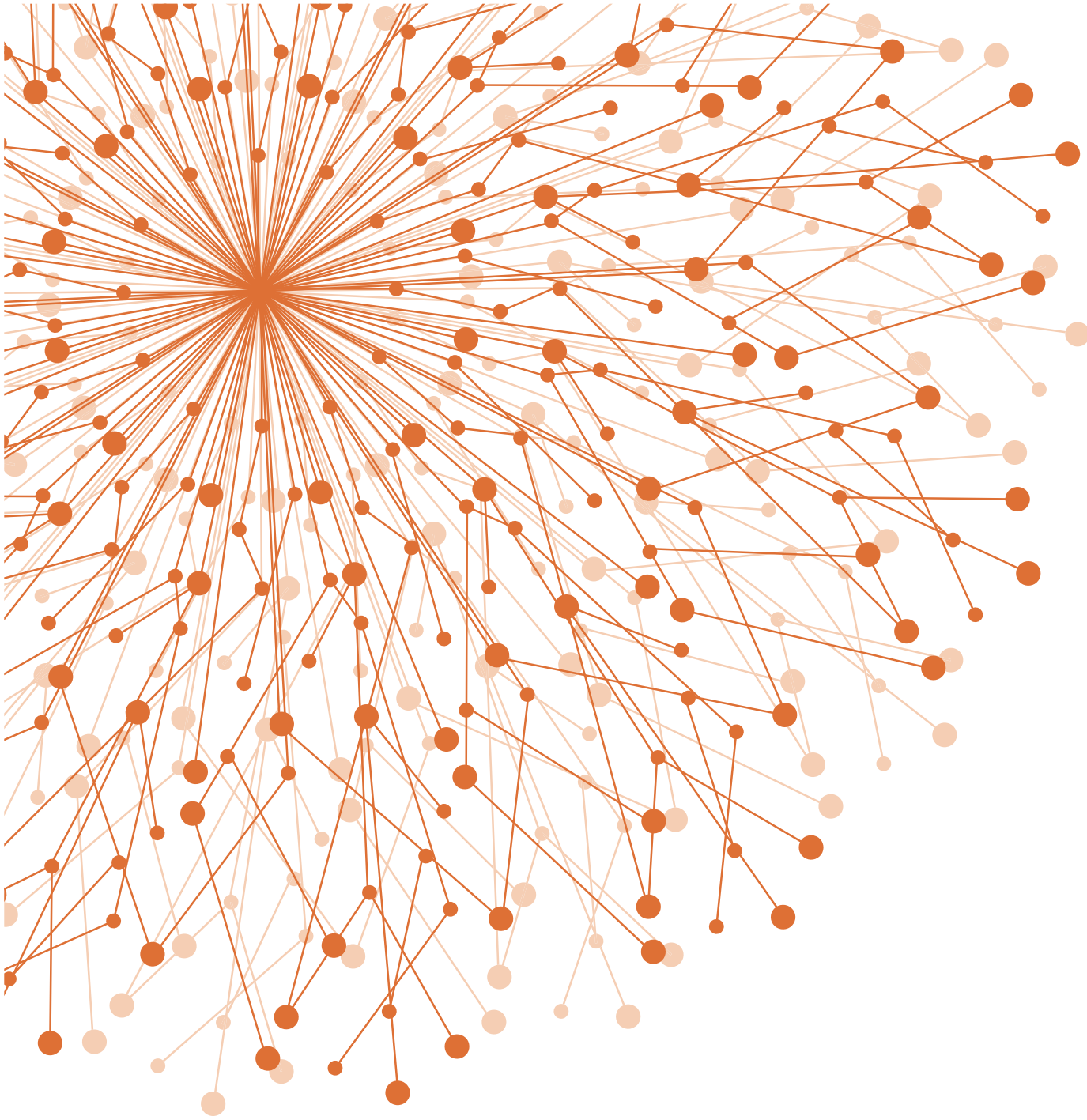

2022 AIChE ANNUAL MEETING

November 13-18, 2022
Phoenix Convention Center
Phoenix, AZ

>POWERING **THE FUTURE**

2022 AIChE ANNUAL MEETING
POWERING THE FUTURE
NOVEMBER 13-18, 2022 • PHOENIX, AZ

TECHNICAL SESSIONS 2022

(1) Workshop: Career Planning for Prospective Faculty

Sunday, Nov 13, 10:00 AM
Phoenix Convention Center, N-227C

Timothy Anderson, Chair
Geoffrey Prentice, Co-Chair

Sponsored by: Career Guidance Committee Liaison

10:00: Welcoming Remarks

10:05: Workshop

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

Sunday, Nov 13, 1:00 PM
Phoenix Convention Center, North Hall E

Roman Voronov, Chair
Sundararajan Madihally, Co-Chair

Sponsored by: Meet the Candidates Poster Sessions

Poster 2a: Engineering Nanostructured Soft Materials for Electrochemical Processes — ***Zhongyang Wang***

Poster 2b: Model-based analysis of CO2 separation processes with various isotherm shapes — ***Yuya Takakura***

Poster 2c: Towards a New World of Plastic Processing & Recycling Via Advanced Reactor Technologies — ***Ali Zolghadr***

Poster 2d: Modeling interspecies competition and exchanges in microbial communities — ***Andrew Freiburger***, *Fatima Foflonker, Jeffrey Dewey, Gyorgy Babnigg, Dionysios Antonopoulos, Christopher S. Henry*

Poster 2f: Exploring Fractal Canyons in Glassy Energy Landscapes — ***Amruthesh Thirumalaiswamy***, *Robert Riggleman, John C. Crocker*

Poster 2g: Surface Chemistry for Efficient Charge Transfer in Hybrid Energy Conversion Systems — ***Ke Ma***

Poster 2h: Designing Active Biomaterials through Multifunctionality of Stimuli-Responsive Polymers — ***Tayler Hebner***

Poster 2j: Leveraging Linked Organ-on-a-Chip Platforms to Study Gut Microbiome Effects on Human Health and Disease — ***Danielle Brasino***

Poster 2k: Leveraging Thermal and Electrocatalysis for Decarbonization of the Energy and Chemical Industries — ***Jason S. Bates***

Poster 2l: Engineering and Applications of Molecularly Assembled Architected Soft Materials — ***Kaiwen Hsiao***

Poster 2m: Bioresorbable Batteries for Self-Powered Bioelectronics and Medical Devices — ***Yamin Zhang***, *John A. Rogers*

Poster 2n: Bridging Length Scales for Correlative and Data Science-Augmented Characterization of Energy Materials — ***Saman Moniri***

Poster 2o: Fundamental Catalytic Reaction Design for Sustainable and Green Chemical Engineering — ***Qiaowan Chang***

Poster 2p: Connecting Computational Chemistry and Its Applications at All Scales - from *Ab Initio* Quantum Chemistry to Continuum Modeling — ***Rui Xu***

Poster 2q: Ion-Mediated Manufacturing of Dynamic Nanostructured Polymer Materials — ***Shuyi Xie***

Poster 2s: How Physicochemical Forces Shape Microbial Recombination in the Host Environment — ***Asher Preska Steinberg***

Poster 2u: Converting Low-Rank Hydrocarbon Wastes into Valuable Anisotropic Carbon Material Intermediates: Combining Experimental Investigation and Data Science — ***Wenjia Wang***

Poster 2v: Interacting Polymer Mixtures for Health and the Environment — ***Scott Danielsen, PhD***

Poster 2w: Nanoengineering of Colloidal Soft Matter Towards Optical and Biological Applications — ***Fan Cui***

Poster 2x: Transient Spectro-Kinetic Approach: A Tool for Deciphering Complex Structure-Function Relationships in Heterogeneous Catalysis — ***Sagar Sourav***

Poster 2y: Process Intensification for Electrochemical Manufacturing — ***Bertrand J. Neyhouse***

Poster 2z: Towards an Atomistic Understanding of Microenvironment Effects in (electro)Catalytic Reactions for Energy Conversion — ***Nitish Govindarajan***

Poster 2aa: Optimization-Based Assessment Framework for Identification of the Optimal CO_2 Utilization Strategy to Energy Products — ***Chanhee You***, *Minseong Park, Hegwon Chung, Jiyong Kim*

Poster 2ab: Enzymatic Synthesis and Metabolism of Small Molecules — ***Karthik Sankaranarayanan***

Poster 2ac: Understanding and Improving Supported Metal Oxide Catalysts — ***Sol Ahn***

Poster 2ad: Developing a Sustainable and Scalable Platform of High-Performance Degradable Polymers — ***Lorenz Manker***

Poster 2ae: Molecular-Based Modeling of Polymer Dynamics for Material Design and Processing — ***Marat Andreev***

Poster 2af: Leveraging Molecular Designs for Colloidal Platforms with Tunable Structures and Properties — ***Hojin Kim***

Poster 2ag: Decarbonizing Chemical Manufacturing: CO_2 Capture & Utilization from Point Sources and Electrochemical Synthesis of Chemicals Using Renewable Energy — ***Nishithan Balaji Chidambara Kani***

Poster 2ai: Battery Materials Harvesting — ***Lingping Kong***

Poster 2aj: Enabling Technologies for Point-of-Care Diagnostics and Targeted Drug Delivery — ***Mohammad Mofidfar***

Poster 2ak: Resisting Dendrites in Lithium Batteries, One Pinhole at a Time — ***Solomon Oyakhire***

Poster 2al: Engineered Multiscale Materials from Biopolymers for Sustainable Agriculture and Manufacturing — ***Muchun Liu***

Poster 2am: Reaction Engineering of Complex Systems (RECS): Towards Circularity and Sustainability — ***SriBala Gorugantu***

Poster 2an: CO_2 Hydrogenation Reaction over Pd-Containing MWW Zeolite Catalyst — ***Willie Yang***, *Shuhei Yasuda, Sridharan Balu, Toshiyuki Yokoi*

Poster 2ao: Nanoporous Materials for Energy, Healthcare, and Sustainability — ***Kaihang Shi***

Poster 2ap: Self-Discharge in Electrochemical Capacitors: Beyond Conway's Diagnostics — ***Deeksha N V N***, *Ganesh Madabattula, Sanjeev Kumar*

Poster 2aq: Nucleic Acid Detection By Target-Assisted Synthesis of Enzyme Reporters in a Cell-Free Protein Synthesis System — ***Yu Jin Park***, *Dong-Myung Kim*

Poster 2ar: Designing Granular Hydrogels for Bioengineering Applications — ***Victoria Muir***

Poster 2as: Engineering Macrophages and Biomaterials to Overcome Barriers in Immunotherapies and for Novel Biomedical Applications — ***Lawrence J. Dooling***

Poster 2at: Tailored Polymeric Systems: Material Properties Informed By Molecular Design — ***Caitlin Sample***

Poster 2au: Design and Control of Biological Assemblies By Leveraging Self-Organization — ***Krishna Shrinivas***

Poster 2av: Next-Generation Materials through Sustainable Polymer Synthesis and Processing — ***Jeffrey Self***

Poster 2aw: Genetically Engineered Commensal Bacteria As Theranostic Probes for the Lungs — ***Michael Brasino***

Poster 2az: Understanding Nanomaterials for Biosensors and Catalysts — ***Anuja Tripathi***

Poster 2ba: Biomolecular Interactions and Transport Laboratory (BIT Lab) to Create a Transformative Impact on Human Health. — ***Aditya Raghunandan***

Poster 2bb: Data-Driven and Physics-Based Methods for Atomistic Modeling of Electrochemical Interfaces — ***Siddharth Deshpande***

Poster 2bc: Design of Heterogeneous Catalysts for Energy Conversion Reactions — ***Md Delowar Hossain***

Poster 2bd: Developing Catalysts for Solar-Driven Chemicals, Fuel Production, and Waste Water Treatment — ***Aisulu Aitbekova***

Poster 2be: Supporting the Circular Economy and Advanced Manufacturing through Soft-Matter Simulations and Theory — ***Benjamin Dolata***

Poster 2bf: Bridging Thermal and Electrochemical Catalysis: Rational Catalyst Design at Atomic Scales through Physical and Machine Learning Based Insights — ***Shyam Deo***

Poster 2bg: Green Organic Photoredox Catalysis: Electronic Structure Guided Design and Discovery — ***Kareesa Kron***, *Andres Rodriguez-Katakura, Rachelle Elhessen, Maria Reed, J. Ryan Hunt, Jahan Dawlaty, Shaama Mallikarjun Sharada*

Poster 2bh: Light-Tunable Two-Dimensional Nanopore for Energy-Efficient Separation — ***Shiqi Huang***

Poster 2bi: An Information-Driven Approach for Controlling Emergent Order in Soft Materials — ***Ashley Guo***

Poster 2bj: Machine Learning-Assisted Materials Design for Energy and Sustainability — ***Yasemin Basdogan***

Poster 2bk: Using Machine Learning to Empower Science and Strengthening Machine Learning through Physics — ***Matthew Spellings***

Poster 2bl: Guiding the Development and Deployment of Sustainable Energy Systems with Data-Informed Modeling of Energy and Chemical Technologies — ***Micah Ziegler***

Poster 2bm: Advancing Crystallization to Enable Challenging Separations — ***Matthew McDonald***

Poster 2bn: Utilizing Differences in Electronic Structure of Molecules for Improved Metals Separations — ***Subhajyoti Chaudhuri***, *Alexander Weberg, Eric Schelter, George C. Schatz*

Poster 2bo: Post-Doc Candidate: In Vitro Platforms for Biotherapeutic Screening — ***Paulina Babiak***

Poster 2bq: The Role of Extracellular Matrix Viscoelasticity and Confinement on Cell Migration: A Multiscale Bio-Chemo-Mechanical Model — ***Wenya Shu***

Poster 2br: Elucidate the Role of Membrane-Bound Organelle Interactome in Parkinson's Disease — ***Han Zhao***

Poster 2bt: Comparative Analysis of Cell-Free Synthesis Systems Based on the Extracts Different Microorganisms. — ***So Jeong Lee***, *Seong-Joo Hong, Choul-Gyun Lee, Yungyu Lee, SangWoo Seo, Dong-Myung Kim*

Poster 2bu: MOFs-Derived Carbon (MDC) for Organic Chloride Removal in the Waste Plastic Pyrolysis Oil (WPPO) and Its Modeling Studies (Kinetic, equilibrium, and thermodynamic analysis) — ***Seong Cheon Kim***, *Dasom Jeong, Siyoung Q. Choi, Jeasung Park*

Poster 2bv: Harnessing Hydrogen Transfer in Energy Science to Boost Sustainability — ***Gang Wan***

Poster 2bw: Improving the Understanding of Dynamics and Mechanical Response of Mixed Moduli Polymer Materials through Simulation — ***Joshua Mysona***

Poster 2bx: Accelerated Discovery of Polymer Materials and Chemical Reactions — ***Dylan Walsh***

Poster 2by: Engineering Instructive Vascular Tissues As Biological Models and Next-Generation Therapies — ***Mai T. Ngo***

Poster 2bz: Colloidal Soft Materials Driven By Electromagnetic Fields — ***Zachary Sherman***

Poster 2ca: Optimization of Concentric-Tube Internal Loop Airlift Photobioreactors for Commercial-Scale Microalgae Cultivation Using Multiphysics Simulations — ***Lifeng Li***, *Xiaoyun Xu, Wujun Wang, Raymond Lau, Chi-Hwa Wang*

Poster 2cb: Development of an Integrated Multiscale Modeling, and Control Framework for Commercialization of Quantum Dot Manufacturing and Their Applications — ***Niranjan Sitapure***, *Joseph Kwon*

Poster 2cc: Model-Based Process Design — ***Ayse Eren***

Poster 2cd: Single-Particle/Molecule Tracking to Probe Transport in Confined Environments — ***Haichao Wu***

Poster 2ce: Biomaterial Strategies to Modulate Immunity for Disease Amelioration — ***Apoorv Shanker***

Poster 2cf: An Epitrochoidal Rotary Reactor for Solar Hydrogen Production Via Ceria Redox Cycle — ***Bo Wang***

Poster 2ch: Unraveling Self-Discharge Mechanisms in Electrical Double-Layer Capacitors (EDLCs) — ***Deeksha N V N***, *Ganesh Madabattula, Sanjeev Kumar*

Poster 2ci: Optical Recording of Bioelectrical Signals Harnessing Bio-Electrochromic Materials Interface — ***Yuecheng Peter Zhou***

Poster 2cj: Improving the Performance of Hollow Fiber Membrane for Energy-Efficient Water Purification — ***Shahriar Habib***

Poster 2ck: Dual-Modal Flexible Operation of on-Site Hydrogen Refueling Station — ***Minseong Park***, *Chanhee You, Hegwon Chung, Jiyong Kim*

Poster 2cl: Experimental and Theoretical Investigations on Electrochemical Removal of Reactive Black 5 Dye from Wastewater — *Kajal Gautam,* ***Sushil Kumar***, ***Dipesh Patle***, *Suantak Kamsolian, Vishwajeet P. Singh*

Poster 2cm: To be Added.

Poster 2cn: Development and Implementation of Organic Color Center Nanosensors for Biomedical Applications — ***Mijin Kim***

Poster 2co: Towards Rational Design of Structured Soft Earth Materials — ***Shravan Pradeep***

Poster 2cp: Interdisciplinary Research to Advance Flow-Based Electrochemical Power Systems — ***Nicholas Cross***

Poster 2cq: Chemical Informatics-Directed Modeling and Processing of Polymeric Materials — ***Weizhong Zou***

Poster 2cr: Synergizing Molecular Simulations and Machine Learning for Understanding Molecular Interactions. — ***Xinqiang Ding***

Poster 2cs: New Catalytic Pathways Towards Waste to Chemicals Conversion and Sustainable Manufacturing — ***Pavel Kots***

Poster 2cu: Computer-Aided Molecular Design: Combining Knowledge-Based and Data-Driven Approaches — ***Ye Seol Lee***

Poster 2cv: Rational Design of Ion Exchange Membranes for Sustainable Water and Energy — ***Jung Min Kim***

Poster 2cw: Voltage As a Driving Force for Sustainably Forming Chemical Bonds — ***Zachary Schiffer***

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Poster 2cy: Computational Assessment of Catalytic Materials — ***Alexander Hoffman***

Poster 2cz: Understanding Ion Transport and Thermodynamics in Electrochemical Systems for Energy and Separations — ***Oscar Nordness***

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Poster 2db: Influence of pH on the Capture Efficiency and Deposition Patterns in an Evaporating Sessile Droplet with Antibody Antigen Surface Reaction — ***Vidisha Singh Rathaur***, *Nachiket Ashish Gokhale, Siddhartha Panda*

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Poster 2dd: Synthetic, Orthogonal Metabolic Pathways for Sustainable Bioconversion and Biomanufacturing of Industrially Relevant Chemicals — ***Seung Hwan Lee***, *Ramon Gonzalez*

Poster 2de: Belowground Carbon Farming: Engineering Genetic Circuits in Plant Roots and Rhizobacteria for Soil Carbon Input — ***Christopher Dundas***

Poster 2df: Autonomous Labs to Accelerate Discovery and Understanding of Organic Mixed Conducting Materials — ***Martin Seifrid***

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Poster 2dl: Elucidating the Mechanical and Transport Properties of Novel Composite Hydrogels Containing Fractionated, Purified Lignin — ***Nicholas Gregorich***, *Sagar Kanhere, Graham W. Tindall, Jaden Stutts, Keturah Bethel, Junhuan Ding, Tyler Martin, Amod Ogale, Mark C. Thies, Eric M. Davis*

Poster 2dn: Developing High-Throughput Tools for Functional Macromolecular Design — ***Melody Morris***

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Poster 2hx: Comparison of Decarbonization Effectiveness Among Steelmaking, Cement, and Aluminum Sectors — ***Lingyan Deng***, *Sydney Johnson, Emre Gençer*

Poster 2hz: Leveraging Membrane Biophysical Features for Enhanced Functionality of Cell-Mimetic Systems — ***Justin Peruzzi***

Poster 2ib: Oxidative Coupling of Methane: Developing Structure-Property Relationships for High-Performance Metal Oxide Catalysts — ***Mariano D. Susman***, *Matteo Ferri, Raffaele Cheula, Hien N. Pham, Abhaya Datye, Sivadinarayana Chinta, David West, Matteo Maestri, Jeffrey Rimer*

Poster 2ic: Role of New Class Functionalized Ionic Liquids for Enhancement of CO2 Capturing Performance of N-Methyldiethanolamine: Kinetics Study and Interaction Mechanism Analysis — ***Surya Tiwari***

Poster 2id: Integrating across Scales in Computational Protein Engineering — ***Tucker Burgin***, *David Beck, Jim Pfaendtner*

Poster 2ie: Interfacing Synthetic Biology with Electrochemistry and Biomolecular Condensate — ***Yifan Dai***

Poster 2if: Enhancing the Bioconversion of Major Lignocellulosic Fractions to Medium Chain Length-Polyhydroxyalkanoates — ***Jorge Arreola Vargas***, *Xianzhi Meng, Yun-Yan Wang, Arthur Ragauskas, Joshua Yuan*

Poster 2ig: Manipulating and Chaining Polyelectrolyte Droplets with an Electric Field — ***Aman Agrawal***, *Matthew V. Tirrell, Jack F. Douglas, Alamgir Karim*

Poster 2ih: Data Science Enabled Cell Analysis for Improving Pre-Clinical to Clinical Translation Pipelines — ***Hawley Helmbrecht***, *Elizabeth Nance*

Poster 2ij: Enhanced Electrochemical Struvite Precipitation from Phosphate-Rich Wastewater Using Pulsating Voltage — ***Ruhi Sultana***, *Lauren F. Greenlee*

Poster 2ik: Investigating Non-Equilibrium Forcing in Biological Tissues and Design of Bio-Inspired Active Adaptive Materials — ***Yuqing Qiu***

Poster 2il: Howsmon Laboratory: Systems Biology and Biomedical Signals — ***Daniel P. Howsmon***

Poster 2im: Toward a More Sustainable World with Heterogeneous Photocatalysis: From Bench to Industry — ***Hossein Robatjazi***

Poster 2in: Theory and Design of Non-Natural Peptides That Undergo Folding-Induced Self-Assembly to Liquid-Liquid Phase Separation. — ***Nairiti Sinha***, *Craig J. Hawker, Matthew Helgeson*

Poster 2io: Bending the Drug Delivery Paradigm By Targeting Nanocarriers for Accumulation within the Body's Intrinsic Barriers — ***Nicholas Lamson***

Poster 2ir: Computational Modeling of Advanced Materials for Sustainable Energy Conversion and Storage — ***Nick Singstock***

Poster 2is: Engineering Single Shot Vaccine Platform Comprising Liposome Embedded Polyelectrolyte Nanofilms Assembly for Controlled Release of Inactivated Chikungunya Virus — ***Rashi Porwal****, Anuj Sharma, Srivatsan Kidambi*

Poster 2it: Scalable Decision-Making for Decarbonized Energy Systems — ***Sungho Shin***

Poster 2iu: Rheological (Structural) and Interfacial Properties of Emulsions and Foams for Environmental Applications — ***Muchu Zhou****, Reza Foudazi*

Poster 2iv: Advanced Membrane Designs and Fundamentals at the Water-Energy Nexus — ***Mahsa Abbaszadeh***

Poster 2iw: Intricacies of Spontaneous Emulsification — ***Monicka Kullappan****, Wesley D. Patel, Manoj K. Chaudhury*

Poster 2iy: Dual Stimuli-Responsive Polycationic Nanoparticles for miRNA Delivery in the Treatment of Glioblastoma Multiforme — ***Deidra Ward***

Poster 2iz: Interdroplet Interactions and Rheology of Nanoemulsion Templates for Synthesis of Porous Hydrogels — ***Zahra Abbasian Chaleshtari****, Reza Foudazi*

Poster 2ja: Molecular-Level Understanding and Design of Functional Nanomaterials for Sustainable Energy Applications — ***Zachariah Berkson***

Poster 2jb: Low-Cost and Membrane-Free Chloride Redox Flow Battery with Multiphase Flow — ***Singyuk Hou****, Chunsheng Wang*

Poster 2jc: Accelerating the Transition Towards a Sustainable Bioeconomy through an Integrated Biorefinery Development Framework — ***Yoel Cortes-Pena****, Jeremy Guest*

Poster 2jd: Probing the Mechanism of Isonitrile Formation By a Non-Heme Iron(II)-Dependent Oxidase/Decarboxylase — ***Antonio Del Rio Flores****, Wenjun Zhang*

Poster 2je: Polymer Membrane Technology, Synthesis of Copolymer Membrane with Polystyrene and Divinylbenzene Used in Electrodialysis and It's Applications — ***Rajni Bala Talwar***

Poster 2jh: Machine-Learned Committor Functions for Reactive Molecular Dynamics — ***Jacob Gissinger***

Poster 2ji: Using analytical and computational chemistry to uncover chemical mechanisms of complex systems — ***Heather LeClerc***

Poster 2jj: Platinum nanoparticles encapsulated within PLGA, treatment for TNBC, an *in vitro* and *in vivo* study. — ***Aida López Ruiz***

Poster 2jk: Engineering Cytokines for the Treatment of Metabolic Diseases — ***Lisa Volpatti***

Poster 2jl: Coarse-Grained Simulation of Self Healing Supramolecular Polymers with Highly Branched Architectures — ***Cody Bezik****, Amalie Frischknecht*

Poster 2jm: Exploiting Light-Matter Interactions for Renewable Chemical Production — ***Steven Anthony Chavez***

Poster 2jn: Colloidal science and macromolecular interactions: Leveraging soft materials in medicine and sustainability — ***Amir Erfani***

Poster 2jo: Influence of Bifunctional PtZn/SiO_2 and H-ZSM-5 on the Rates and Selectivity of Propene Aromatization — ***Christopher Russell***

Poster 2jp: Surface Redox Mediators Co-catalyze the Reduction of O2 to H2O2 on Pd Nanoparticles — ***Jason S. Adams****, Ashwin Chemburkar, Mayank Tanwar, Pranjali Priyadarshini, Tomas Ricciardulli, Vineet Maliekkal, Sucharita Vijayaraghavan, Yubing Lu, Abinaya Sampath, Ayman M. Karim, Matthew Neurock, David Flaherty*

Poster 2jq: Exploring Protein/Polymer Interactions in Biotechnology Applications — ***Antonio Dos Santos***

Poster 2jr: Molecular Engineering of Advanced Polymeric Materials for Energy and Sustainability — ***Anthony Engler***

Poster 2js: Engineering Biological Systems for Climate Resilience and Human Health: From Proteins to Ecological Communities — ***Tejas Navaratna***

Poster 2jt: Advanced Membrane Separations as a Teaching-Focused Faculty Member — ***Maura Sepesy****, Christine Duval*

Poster 2ju: *Developing frugal and sustainable techniques for addressing the health issues arising from legacy and emerging nano-contaminants* — ***Laxmicharan Samineni***

Poster 2jv: Multifunctional Engineered Living Materials from Bacteria — ***Sara Molinari***

Poster 2jw: Design Principles for Active Matter Materials — ***Tingtao Zhou***

Poster 2jx: Charge based high throughput fractionation and biosensing of exRNA nanocarriers (Extracellular vesicles, Lipoproteins and Ribonucleic protein) — ***Himani Sharma***

Poster 2jy: Tuning the Interface for Carbon Dioxide Removal Chemistries with First Principles Computational Methods — ***Colin Ling Chong***

Poster 2jz: Elucidating the role of network topology dynamics on the coil-stretch transitionhysteresis in extensional flow of entangled polymer melts — ***Mahdi Boudaghi***

Poster 2ka: Molecular Simulation of Mechanical Effects of Adsorption in Gas and Liquid Phase — ***Alina Emelianova***

Poster 2kb: Cell-free Engineering of Photosynthesis for Chemical and Energy Production — ***Blake J. Rasor***

Poster 2kc: Advances in Fuel Properties, Production and Processing — ***M R Riazi***

Poster 2kd: Protein evolution: a bridge between basic discoveries and applications — ***Monica Neugebauer***

Poster 2ke: Sustainable Materials and Process Design through Multi-Scale Systems Engineering and Hybrid Mechanistic/Data-Driven Modeling — ***Kazi Khoda***

Poster 2kf: End-to-End Design of Nematicity, Chirality, and Charge in Biopolymers *via* Molecular Simulation and Machine Learning — ***Kevin Shen***

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(3) Discussing the 2022 NASEM Report: New Directions for Chemical Engineering

Sunday, Nov 13, 3:00 PM
Phoenix Convention Center, N-124AB

Phillip Westmoreland, Chair
Joan Brennecke, Co-Chair

Sponsored by: Research and New Technology Committee (RANTC)

3:00: Introductory Remarks from AIChE President, Christine Grant

3:05 Paper 3a: Invited Talk - Eric Kaler

3:45 Paper 3b: Invited Panel Discussion on NASEM Report — ***Jean Tom****,* ***Cato Laurencin****,* ***Jodie Lutkenhaus****,* ***John Siirola***

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(4) A Celebration of H. Scott Fogler's Life (Invited Talks)

Sunday, Nov 13, 3:30 PM
Phoenix Convention Center, N-129AB

Michael Senra, Chair
Karsten E Thompson, Co-Chair
Ryan Hartman, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

3:30 Paper 4a: The Many Contributions of Scott Fogler to the Chemical Engineering Community — ***Ronald Larson***

3:55 Paper 4b: Scott Fogler – Original Thinker, Leader, Mentor and Dear Friend — ***Maria Burka***

4:20 Paper 4c: H. Scott Fogler - UM Computing, Interactive Teaching, and CACHE — ***Warren Seider***

4:45 Paper 4d: Reflections on Learning from and Teaching with H. Scott Fogler — ***Michael Senra***

5:10 Paper 4e: Graduate Education, Creative Problem Solving, and the Legacy of Scott Fogler — ***Michael P. Hoepfner***

5:35: Open Mic Session: Audience Reflections on H. Scott Fogler

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(5) Dynamic and Transient Reactor Operation

Sunday, Nov 13, 3:30 PM
Phoenix Convention Center, N-127C

Omar Abdelrahman, Chair
Andrew R Teixeira, Co-Chair

Sponsored by: Reaction Engineering

3:30 Paper 5a: Microkinetic Investigation of the Transient CO_2 Methanation on Ni Catalysts in a Berty Reactor — ***Bjarne Kreitz***, *Thomas Turek, C Franklin Goldsmith*

3:48 Paper 5b: Propene Ammoxidation By Bismuth Molybdate Using Forced Dynamic Operation — ***Zhuoran Gan***, *Lars Grabow, William Epling*

4:06 Paper 5c: Programmable Catalysts Control Reaction Selectivity Via Kinetics — ***Sallye Gathmann***, *M. Alexander Ardagh, Paul Dauenhauer*

4:24 Paper 5d: Pi-Criterion Analysis of Non-Steady State Catalytic Oxidation Reactions — ***Austin Morales***, *Praveen Bollini, Michael Harold*

4:42 Paper 5e: Tuning Catalytic Activity with Forced Dynamic Operation — ***Yu Liu***, *Lars Grabow*

5:00 Paper 5f: Controlled Temperature Dynamics in a Catalytic Microreactor — ***Cameron Armstrong***, *Fatou Baka Diop, Andrew R Teixeira*

5:18 Paper 5g: Process Alternatives to Stabilize Small-Scale Ammonia Production. — ***Laron Burrows***, *George M. Bollas*

5:36 Paper 5h: Mechanocatalytic Ammonia Synthesis over TiN in Transient Microenvironments — ***Karoline Hebisch***, *Andrew Tricker, Erin V. Phillips, Jacob A. Dewitt, Marco Buchmann, Yu-Hsuan Liu, Marcus Rose, Eli Stavitski, Andrew Medford, Marta Hatzell, Carsten Sievers*

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(6) In Honor of Norbert Kruse's Birthday (Invited Talks)

Sunday, Nov 13, 3:30 PM
Phoenix Convention Center, N-127B

Jean-Sabin McEwen, Chair
Miquel Salmeron, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

3:30 Paper 6a: Hydrogenation of Functionalized Molecules in Presence and Absence of External Electric Potential — ***Johannes Lercher***

3:50 Paper 6b: Analysis and Prediction of Reaction Kinetics Using the Degree of Rate Control — ***Charles Campbell***

4:10 Paper 6c: The SMSI Effect of Coox-Pt and Coox-Au Inverse Catalysts — ***Miquel Salmeron***

4:30 Paper 6d: Unraveling the Remarkable Stability of Pt-Pd Nanoparticles during Diesel Oxidation Catalysis — ***Abhaya K. Datye***, *Stephen Porter, Hien N. Pham, Arnab Ghosh*

4:50 Paper 6e: Thermally Stable and Highly Active Single Rh Atom Catalysts (Rh_1/ceria) for NO Reduction — ***Yong Wang***

5:10 Paper 6f: Light Alkanes Transformation through Ammonia-Assisted Reforming — ***Yizhi Xiang***, *Siavash Fadaeerayeni*

5:25 Paper 6h: Elucidating the Influence of Electric Fields on Fe Oxidation Via Multiscale Models and Atom Probe Tomography — *Naseeha Cardwell, Sten Lambeets, Isaac Onyango, Yong Wang, Thierry Visart De Bocarmé, Daniel Perea,* ***Jean-Sabin McEwen***

5:45 Paper 6i: A Unique Example of Thermokinetic Oscillations in Heterogeneous Catalysis: The Fischer-Tropsch Reaction over Co/Ce-Oxide Catalysts — ***Norbert Kruse***

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(7) Microporous and Mesoporous Materials I: Catalytic Sites

Sunday, Nov 13, 3:30 PM
Phoenix Convention Center, N-128A

Nicholas Brunelli, Chair
Eleni Kyriakidou, Co-Chair
Steven Saunders, Co-Chair

Sponsored by: Catalysis

3:30 Paper 7a: Catalytic Cycles and Deactivation Mechanisms for Styrene Oxidation over First-Row Transition Metal Carboxylate MOFs — ***Rachel A. Yang***, *Michele Sarazen*

3:48 Paper 7b: Effect of Reaction Conditions and SO2 Exposure on Cu Speciation in SSZ-13 Zeolites — ***Keka Mandal***, *Yu-Ren Chen, Rohil Daya, William Epling, Christopher Paolucci*

4:06 Paper 7c: Kinetic Assessments of the Influence of Active Site Distribution in Brønsted Acid Zeolites on Toluene Methylation Catalysis — ***Sopuruchukwu Ezenwa***, *Rajamani Gounder*

4:24 Paper 7d: Benzene Alkylation with Light Alkenes on Acidic Mordenite: The Effects of Acid Size Locations and Confinements on Reaction Mechanisms — *Hanna Monroe,* ***Stephanie Kwon***

4:42 Paper 7e: Speciation, Siting, Evolution, and Methane Activation Properties of Mo-Oxide-Impregnated H-ZSM-5 Catalyst Precursors for Methane Dehydroaromatization — ***Fateme Molajafari***, *Emanuele Joy, Adriano Brago, Rachita Rana, Ambarish Kulkarni, Simon Bare, Sheima J. Khatib, Joshua Howe*

5:00 Paper 7f: Distributions of Al Atoms in Chabazite Zeolite Frameworks and Their Effects on Adsorption and Catalytic Reaction Properties — ***Michael Schmithorst***, *Ahmad Moini, Subramanian Prasad, Bradley F. Chmelka*

5:18 Paper 7g: Mechanistic Analysis of CO Oxidation over Mixed-Valence Oxo-Bridged Trimers — *Jacklyn Hall,* ***Praveen Bollini***

5:36 Paper 7h: Influence of Interactions between Solvent Structures and Reactant Alkyl Groups on Lewis-Acid Catalyzed Epoxidations — ***David Potts***, *Vijaya Sundar Jeyaraj, Ohsung Kwon, Richa Ghosh, Alexander V. Mironenko, David Flaherty*

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(8) Microreaction Engineering

Sunday, Nov 13, 3:30 PM
Phoenix Convention Center, N-128B

Simon Kuhn, Chair
Milad Abolhasani, Co-Chair

Sponsored by: Reaction Engineering

3:30 Paper 8a: Achieving Ultrafast Dynamic Catalytic Operation Using Microcapillary Flow Reactors — ***Fatou Baka Diop***, *Cameron Armstrong, Andrew R Teixeira*

3:50: Break

4:10 Paper 8c: New Insights on Fixed-Bed Reactor Dynamics Via Real-Time Distributed Temperature Sensing — ***Jens Bremer***, *Ronny Tobias Zimmermann, Kai Sundmacher*

4:30 Paper 8d: Quaternary Phase Segmented Flow Format for Biphasic Reactions — ***Amanda Volk***, *Robert Epps, Daniel Yonemoto, Felix N. Castellano, Milad Abolhasani*

4:50 Paper 8e: Accelerated and Scalable Synthesis of Mfu-4l in Flow — ***Suyong Han***, *Sujay Bagi, Soonhyoung Kwon, Husain Adamji, Mircea Dincă, Yuriy Roman*

5:10: Break

5:30 Paper 8g: SBA-16-Mediated Nanoparticles Enabling Accelerated Kinetics in Cyclic Methane Conversion to Syngas at Low Temperatures — ***Yan Liu***, *Lang Qin, Jianhua Pan, Fanhe Kong, Yu-Yen Chen, Jonathan Fan, Liang-Shih Fan, Josh Goetze*

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

Sunday, Nov 13, 3:30 PM
Phoenix Convention Center, N-222B

Mona Minkara, Chair
Frederick de Meyer, Co-Chair
Obioma Uche, Co-Chair
Yamil Colón, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

3:30 Paper 9a: Atomistic-Level Insights into the Interfacial Interactions between Amyloid-Beta and Phospholipid Bilayers for the Treatment of Alzheimer's Disease — ***Bailey Zinger***, *Joel L. Kaar, Kayla Sprenger*

3:45: Break

4:00 Paper 9c: Computational Discovery of Plastic-Binding Peptides for Microplastic Remediation — ***Michael Bergman***, *Xingqing Xiao, Carol Hall*

4:15 Paper 9d: Computational Investigation of Bijels As Separation Systems — ***Marco Tulio Portella***, *Xuan Duy Thao Nguyen, Dimitrios Papavassiliou*

4:30 Paper 9e: Adsorption of Trace Metal Contaminants from Coal-Derived Syngas on Metal Surfaces and Novel Bimetallic Adsorbents — ***Dwijraj Mhatre***, *Divesh Bhatia*

4:45 Paper 9f: Vapor-Liquid Equilibrium and Nucleation Studies of Water from First Principles-Based Machine Learning Models — ***Maria Carolina Nicola Barbosa Muniz***, *Roberto Car, Athanassios Panagiotopoulos*

5:00 Paper 9g: Metastable Liquid-Liquid Criticality in Supercooled Wail Water — ***Jack Weis***, *Athanassios Panagiotopoulos, Pablo Debenedetti*

5:15 Paper 9h: Molecular Dynamics of Ethoxylated Surfactants in Water/N-Heptane Interface — *Arthur M. Luz, Gabriel D. Barbosa,* ***Thiago Jose Pinheiro Dos Santos***, *Carla L. M. Camargo, Frederico W. Tavares*

5:30 Paper 9i: Dynamic Molecular Switching for Environmentally Adaptive Surfaces — ***Nicholas Craven***, *Chris R. Iacovella, G. Kane Jennings, Clare McCabe*

5:45 Paper 9j: Interactions of Cellulosic Oligomers with Different Crystallographic Surfaces of Cellulose Nanocrystals through Molecular Simulation — ***Naveen Vasudevan***, *Dongyang Li, Li Xi*

(10) Advances in Global Optimization

Sunday, Nov 13, 3:30 PM
Phoenix Convention Center, W-101C

Can Li, Chair
Qi Zhang, Co-Chair

Sponsored by: Systems and Process Operations

3:30 Paper 10a: New Results in the Global Minimization of Molecular Potential Energy Functions — ***Anatoliy Kuznetsov***, *Nikolaos Sahinidis*

3:48 Paper 10b: A Novel Algorithm for Constructing Tight Quadratic Underestimators for Global Optimization — ***William Strahl***, *Arvind Raghunathan, Nikolaos Sahinidis, Chrysanthos Gounaris*

4:06 Paper 10c: New Mccormick-Style Convex Relaxations of Implicit Functions in Global Optimization — *Huiyi Cao,* ***Kamil Khan***

4:24 Paper 10d: Exact Penalty Bayesian Optimization: No-Regret Data-Driven Optimization with Unknown Equality and Inequality Constraints — ***Congwen Lu***, *Joel Paulson*

4:42 Paper 10e: Learning to Accelerate the Global Solution of Quadratically-Constrained Quadratic Programs — ***Rohit Kannan***, *Deepjyoti Deka, Harsha Nagarajan*

5:00 Paper 10f: Improving the Tightness of State Relaxations for Global Dynamic Optimization through Refinement with Invariants — ***Jason Ye***, *Joseph K. Scott*

5:18 Paper 10g: Global Dynamic Optimization Using Hardware-Accelerated Programming — ***Robert Gottlieb***, *Matthew Stuber*

5:36 Paper 10h: Global Optimal K-Center Clustering with Millions of Samples — ***Yankai Cao***, *Kaixun Hua*

(11) Data-Driven and Hybrid Modeling for Decision Making

Sunday, Nov 13, 3:30 PM
Phoenix Convention Center, W-101A

M M Faruque Hasan, Chair
Qiugang Jay Lu, Co-Chair

Sponsored by: Information Management and Intelligent Systems

3:30 Paper 11a: A Hybrid Model Feature Relevance Analysis for First-Principle Model Refinement Suggestions — ***Yushi Deng***, *Selen Cremaschi, Mario Eden, Haijing Gao, Shuxing Cheng*

3:47 Paper 11b: X AI-MEG : An Ontology-Based Explanation Generator Via Machine Learning — *Abhishek Sivaram,* ***Venkat Venkatasubramanian***

4:04 Paper 11c: Meta-Modeling-Based Sensitivity Analysis of Hybrid Models — ***Sagar Vinod Lakhwani***, *Mohammed Saad Faizan Bangi, Joseph Kwon*

4:21 Paper 11d: Subspace Based Model Identification for Batch Quality Analysis Using Missing Data Algorithms — ***Nikesh Patel***, *Kavitha Sivanathan, Prashant Mhaskar*

4:38 Paper 11e: Bayesian Optimization for Performance-Oriented Model Learning: An Application to Learning-Based Predictive and Parameter-Varying Control of Cold Plasmas — ***Kimberly Chan***, *Yajie Bao, Javad Mohammadpour Velni, Ali Mesbah*

4:55 Paper 11f: A Computational Study on the Benefits of Decision-Focused Surrogate Modeling — ***Rishabh Gupta***, *Joshua Larson, Qi Zhang*

5:12 Paper 11g: Decision-Making Optimization of Hybrid Energy Management System for Curtailed Renewable Energy through Deep Reinforcement Learning — *Doeun Kang, Dongju Kang, Sumin Hwangbo, Haider Niaz, Wonbo Lee, J Jay Liu,* ***Jonggeol Na***

5:29 Paper 11h: Hybrid Modeling and Optimization of Process Flowsheets Using Bayesian Symbolic Regression — ***Sachin Jog***, *Daniel Vázquez, Gonzalo Guillén-Gosálbez*

5:46 Paper 11i: Data-Driven Explainable Classification for Economic Bioproduct Separation — ***Jianping Li***, *Reid Van Lehn, Christos Maravelias*

(12) Data-Driven Dynamic Modeling, Estimation and Control I

Sunday, Nov 13, 3:30 PM
Phoenix Convention Center, W-101B

Joseph Kwon, Chair
Calvin Tsay, Co-Chair

Sponsored by: Systems and Process Control

3:30 Paper 12a: Active Deep Learning for Scalable Approximation of Reachable and Invariant Sets for Mixed-Integer Nonlinear Systems — ***Joel Paulson***, *Angelo D. Bonzanini, Georgios Makrygiorgos, Ali Mesbah*

3:49 Paper 12b: Development of Mass and Energy Constrained Neural Networks — ***Angan Mukherjee***, *Debangsu Bhattacharyya*

4:08 Paper 12c: Data-Driven Controller Synthesis through the Learning of Integral Quadratic Constraints — ***Wentao Tang***, *Prodromos Daoutidis*

4:27 Paper 12d: Nonlinear Model Predictive Control Using Statistical Machine-Learning-Based Control Lyapunov Barrier Functions — ***Scarlett (Siyao) Chen***, *Zhe Wu, Panagiotis Christofides*

4:46 Paper 12e: Efficient Training of Machine-Learning Enhanced Building Models with Noisy Data — ***Pranav Krishna***, *Matthew Ellis*

5:05 Paper 12f: A Deep Learning-Based Model Reduction and Control of an Ammonia Synthesis Process — ***Thiago Oliveira Cabral***, *Amirsalar Bagheri, Davood Babaei Pourkargar*

5:24 Paper 12g: State Space Model Predictive Control Using Quality Variables for Batch Polymethyl Methacrylate Production — ***Nikesh Patel***, *Prashant Mhaskar*

5:43 Paper 12h: Latent State Space Modeling of High-Dimensional Data in Chemical Systems — *Jiaxin Yu,* ***S. Joe Qin***

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

Sunday, Nov 13, 3:30 PM
Phoenix Convention Center, N-227C

Lisa Bullard, Chair
David Silverstein, Co-Chair
Donald Visco Jr., Co-Chair

Sponsored by: Professional Development Committee Liaison

3:30: Welcoming Remarks

3:35: Workshop

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(14) Fundamentals of Interfacial Phenomena I

Sunday, Nov 13, 3:30 PM
Phoenix Convention Center, N-232B

Dongjin Seo, Chair
Sepideh Razavi, Co-Chair
Younjin Min, Co-Chair
Xiaoguang Wang, Co-Chair

Sponsored by: Interfacial Phenomena

3:30 Paper 14a: Investigation and Analysis of Scattered Light from the Deformation and Adhesion of Synthesis Oil-in-Water Microcapsules — ***Hairou Yu***, *Jiarui Yan, Christopher Wirth*

3:45 Paper 14b: Enhanced Microscale Flow and Controllable Phase Separation in an Evaporating Enzyme-Loaded Aqueous Two-Phase System (ATPS) Droplet — ***Yang Cao***, *Ho Cheung Shum*

4:00 Paper 14c: Surface Functionalization of Different Plastic Substrates with a Hydrophilic/Oleophobic Perfluoropolyether Coating — ***Yihan Song***, *Michaela Dunleavy, Lei Li*

4:15 Paper 14d: Free Energy Analysis of Biomolecule Adsorption to Graphene-Cu(111) and Defective Graphene-Cu(111) Interfaces: Molecular Insights into Biofilm Formation and Adhesion — ***Sourav Verma***, *Kenneth Benjamin*

4:30: Break

4:45 Paper 14f: Linear Response of Finite Thickness Membranes — ***Zachary Lipel***, *Yannick Azhri Din Omar, Kranthi K. Mandadapu*

5:00 Paper 14g: Electromechanics of Lipid Bilayers: A Dimensionally Reduced Theory with Applications — ***Yannick Azhri Din Omar***, *Zachary Lipel, Kranthi K. Mandadapu*

5:15 Paper 14h: Effect of Interfacial Solvent Structures on the Formation of Worm-like Micelles: A Molecular Dynamics Study — *Kaijie Zhang, Mingshan Zhang,* ***Zhehui Jin***

5:30 Paper 14i: Mechanical Stress Sensing with Molecularly Thin Films — ***Tanner Finney***, *Tonya L. Kuhl*

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(15) Rational Design and Optimization of Soft Materials

Sunday, Nov 13, 3:30 PM
Phoenix Convention Center, N-222C

Kathleen McEnnis, Chair
Poornima Padmanabhan, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

3:30 Paper 15a: Entropically Engineered Assembly of Fivefold and Icosahedral Twin Clusters — ***Sangmin Lee***, *Sharon Glotzer*

3:45 Paper 15b: Design of Soft Pair Potentials for Mesophase Formation in DNA Decorated Colloids — ***Luis Nieves Rosado***, *Fernando Escobedo*

4:00 Paper 15c: Computational Study of Mechanochemical Activation in Nanostructured Triblock Copolymers — *Zijian Huo, Stephen Skala, Jennifer Laaser,* ***Antonia Statt***

4:15 Paper 15d: Multi-Fidelity Computational-Experimental Design of Self-Assembling π-Conjugated Peptides — ***Kirill Shmilovich***, *Sayak S. Panda, Anna Stouffer, John D. Tovar, Andrew Ferguson*

4:30 Paper 15e: Solvation Against Polarity: A Simulation Study on Mixed-Polarity Grafted Polymer Electrolytes — ***Chuting Deng***, *Peter Bennington, Paul F. Nealey, Shrayesh Patel, Juan De Pablo*

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(16) Self-Assembly in Solution

Sunday, Nov 13, 3:30 PM
Phoenix Convention Center, N-232A

Po-Yen Chen, Chair
Paschalis Alexandridis, Co-Chair
Javen Weston, Co-Chair

Sponsored by: Interfacial Phenomena

3:30 Paper 16a: Snagging mRNA in Wormlike Micelle Networks — *Kimberly Hui, Kyle J. Tynan,* ***James W. Schneider***

3:45 Paper 16b: Role of Chain Architecture on the Solution Phase Assembly and Thermoreversibility of Aqueous PNIPAM/Silyl Methacrylate Copolymers — *Jason D. Linn, Lucy Liberman,* ***Michelle Calabrese***

4:00 Paper 16c: Morphological and Rheological Transitions of Zwitterionic Surfactant Based pH-Tunable Dynamic Binary Complex Coacervates — ***Bhargavi Bhat***, *Silabrata Pahari, Shuhao Liu, Yu-Ting Lin, Joseph Kwon, Mustafa Akbulut*

4:15 Paper 16d: Probing Microstructure of Self-Assembled Micellar Solutions Via 1D ^{1} h NMR Diffusometry — ***Alfredo Scigliani***, *Samuel Grant, Hadi Mohammadigoushki*

4:30 Paper 16e: Synergistic Effects of Surfactant Mixtures on Micellization and on Adsorption at Interfaces — ***Kristo Kotsi***, *Teng Dong, Takeshi Kobayashi, Ian McRobbie, Alberto Striolo, Panagiota Angeli*

4:45 Paper 16f: Catanionic Surfactant Self-Assembly System Assessed from Membrane Properties — ***Nozomi Watanabe***, *Syuto Watase, Nanaki Kadonishi, Yukihiro Okamoto, Hiroshi Umakoshi*

5:00 Paper 16g: Pfas Surfactant Association with Cyclodextrins — *Yuxin Bao, Samhitha Kancharla, Paschalis Alexandridis,* ***Marina Tsianou***

5:15 Paper 16h: Hydration of Linear Alkanes Is Governed By the Small Length-Scale Hydrophobic Effect — *Himanshu Singh,* ***Sumit Sharma***

5:30 Paper 16i: Disclosing Interior Structure of Nanostructured Lipid Carriers: Relation of Core-Shell Structure to Lipid Composition — ***Nozomi Watanabe***, *Ni'matul Izza, Yukihiro Okamoto, Hiroshi Umakoshi*

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(17) Design and Analysis of Sustainable Carbon Capture and Emissions Control Technologies

Sunday, Nov 13, 3:30 PM
Phoenix Convention Center, N-225B

Gerardo Ruiz-Mercado, Chair
David Miller, Co-Chair

Sponsored by: Fossil Energy

3:30 Paper 17a: Process Analyses of Selective NO_x Decomposition Employing Chemical Looping Scheme — ***Pinak Mohapatra***, *Sonu Kumar, Rushikesh Joshi, Liang-Shih Fan*

3:55 Paper 17c: Techno-Economic Analysis of a Combined Power Plant CO2 Capture and Direct Air Capture Concept for Flexible Power Plant Operation — ***Moataz Sheha***, *Edward Graham, Dharik Mallapragada, Emre Gençer, Phillip Cross, James Custer, Adam Goff, Ian Cormier, Howard Herzog*

4:20 Paper 17d: Evaluation of Aprotic Heterocyclic Anion Ionic Liquids for Post Combustion Carbon Capture — ***Tracy Benson***, *Adhish Chandra Saketh Madugula*

4:45 Paper 17b: Recovery of Vapors and Organic Compounds during Industrial Coffee Roasting — ***Saad Barbar Netto***, *Murilo Innocentini, Cristina Paschoalato, Silvia H. Taleb-Contini,* ***Tapas Das***, *Pedro Pires*

5:10 Paper : Enhanced Elimination of Carbonaceous Gaseous Elements and Coal Dust Particulate Matters from Flue Gas by Using the Fully Submerged Self-Primed Venturi Scrubber — ***Subhrajit Mukherjee***, *Abesh Chatterjee, Bhim Charan Meikap*

(18) Fundamentals of Food, Energy, Water Systems

Sunday, Nov 13, 3:30 PM
Phoenix Convention Center, N-225A

Philip Tominac, Chair
Dhabia Al-Mohannadi, Co-Chair
Debalina Sengupta, Co-Chair

Sponsored by: Fundamentals

3:30 Paper 18a: Microbial Soil Amendments for Modulating Soil Moisture Dynamics for Improved Water Availability in Agriculturally Relevant Soils — ***Moises M. Gutierrez***, *Micah V. Cameron-Harp, Partha P. Chakraborty, Emily M. Stallbaumer-Cyr, Jordan A. Morrow, Ryan Hansen, Melanie M. Derby*

3:55 Paper 18b: An Energy Efficient Nitrogen Removal Process Via Simultaneous Nitrification and Denitrification in Wastewater — *Qingkun Wang,* ***Jianzhong He***

4:20 Paper 18c: Nutrient Recovery from Hydrothermally-Treated Dairy Manure Using Algae Cultivation — ***Callan Glover***, *Nicholas Silva, Gabriela Quiles, Pablo Cornejo, Sage Hiibel*

4:45 Paper 18d: *Assessing the Use of OIL and Gas Produced Water for Soil Aquifer Treatment in ABU DHABI* — ***Hala Alomary***, *Jisha Ali, Abdulfahim Arangadi, Kosmas Pavlopoulos, Daniil Moraitis, Emad Alhseinat*

5:10 Paper 18e: Phytoremediation of Deicing Salt from Roadside Soils — ***Leif van Lierop***, *Bo Hu*

5:35 Paper 18f: Caffeine Removal Using "the Miracle Tree" Wastes for Sustainable Water Purification Processes As Alternative to Classic AOP and Commonly Used Filtration Media — *Israel Sornoza, Alina L. Trávez, Nicole González,* ***Andrea Landázuri***, ***Andres S. Lagos***, *David Egas, Lourdes Orejuela Escobar, Rodny Peñafiel*

(19) Biomolecular Engineering I

Sunday, Nov 13, 3:30 PM
Phoenix Convention Center, N-126A

Xue Sherry Gao, Chair
Whitney Stoppel, Co-Chair
John Blazeck, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

3:30 Paper 19a: Discovery and Characterization of a Novel Lasso Peptide Using a Guilt By Association Approach — ***Drew Carson***, *A. James Link*

3:48 Paper 19b: Rational Design of an Adenosine-Degrading Enzyme for Therapeutic Administration in Tumor Mouse Models — ***Maria Rain Jennings***, *John Blazeck*

4:06 Paper 19c: Peptide Aggregation Induced Immunogenic Rupture (PAIIR) — ***Gokhan Gunay***, *Seren Hamsici, Handan Acar*

4:24 Paper 19d: Recombinant Serine Protease Inhibitors (serpins) for Tissue Repair — ***Jordan Yaron***, *Jayda Hylton-Pelaia, Jordan Roberts, Holly Gildar, Jacquelyn Kilbourne, Liqiang Zhang, Alexandra Lucas, Kaushal Rege*

4:42 Paper 19e: Generating Extended Grnas with Hairpins for Increased CRISPR Editing Specificity — ***Hillary Dimig***, *Ashley Herring-Nicholas, Eric Josephs*

5:00 Paper 19f: Engineering Improved Crispr Repressors for Targeted Mammalian Gene Regulation — ***Andrew Kristof***, *John Blazeck*

5:18 Paper 19g: Invited Talk: Placeholder for the Invited Talk in the Biomolecular Engineering I Session — ***Whitney Stoppel***, *Xue Sherry Gao, Ashish Kulkarni*

(20) Cell and Tissue Engineering: Mechanical Cues and Cell Behavior

Sunday, Nov 13, 3:30 PM
Phoenix Convention Center, N-126B

Panagiotis Mistriotis, Chair
Laurel Hind, Co-Chair
Whitney Stoppel, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

3:30 Paper 20a: Matrix Remodeling Modulates Human Neural Maturation — ***Michelle Huang***, *Julien G. Roth, Renato Navarro, Bauer L. LeSavage, Sarah C. Heilshorn*

3:48 Paper 20b: Stiffness Promotes Metabolic Reprogramming in Primary Hepatocytes — ***Michael Moeller***, *Senthilkumar Thulasingam, Kimberly M Stanke, Madhusudhanan Narasimhan, Srivatsan Kidambi*

4:06 Paper 20c: Directing Multicellular Organization By Varying the Aspect Ratio of Soft Hydrogel Microwells — ***Gayatri Pahapale***, *Jiaxiang Tao, Milos Nikolic, Sammy Gao, Giuliano Scarcelli, Sean X. Sun, Lewis H. Romer, David Gracias*

4:24 Paper 20d: Fluid Viscosity Enhances Breast Cancer Metastasis through Coordinated Activity between Volume-Regulatory and Mechanosensitive Ion Channels — ***Alexander Kiepas***, *Kaustav Bera, Inês Godet, Selma Serra, Anindya Sen, Se Jong Lee, Yuqi Zhang, Daniele Gilkes, Miguel Valverde, Konstantinos Konstantopoulos*

4:42 Paper 20e: Counterintuitive Effect of Fluid Viscosity on Enhancing Cell Motility Via Dynamic Load Response of Actin Network — ***Kaustav Bera***, *Alexander Kiepas, Brent Ifemembi, Konstantin Stoletov, Yizeng Li, Colin D. Paul, Anindya Sen, Se Jong Lee, Panagiotis Mistriotis, Kandice Tanner, John Lewis, Sean X. Sun, Konstantinos Konstantopoulos*

5:00 Paper 20f: A Modular Microfluidic Platform to Study How Fluid Shear Stress Alters Estrogen Receptor Phenotype in Single Breast Cancer Cells — ***Braulio Ortega Quesada***, *Jonathan Cuccia, Rachel Coates, Elizabeth C. Martin, Adam Melvin*

5:18 Paper 20g: Invited Talk: Placeholder for Mechanical Cues and Cell Behavior — ***Whitney Stoppel***, *Panagiotis Mistriotis, Laurel Hind*

(21) Engineering Protein Therapeutics

Sunday, Nov 13, 3:30 PM
Phoenix Convention Center, N-125A

Maryam Raeeszadeh Sarmazdeh, Chair
Jamie Spangler, Co-Chair

Sponsored by: Bioengineering

3:30 Paper 21a: Engineering a High Affinity Cross-Reactive Antibody to Bind VEGF-a and PlGF-2 — ***Samuel Blackman***, *Alison Lee, Ahlam Qerqez, Jennifer Maynard*

3:48 Paper 21b: Engineering Pan-Reactive VEGF Antagonists for Neovascular Eye Diseases — ***Paul Sargunas***, *Jamie Spangler*

4:06 Paper 21c: Discovery and Characterization of Intracellularly Stable hnRNPA2B1 Specific Nanobodies for Live-Cell Imaging and Targeted Protein Degradation — ***Azady Pirhanov***, *Yongku Cho*

4:24 Paper 21d: Directed Evolution of Monoclonal Antibodies Against Tumor Associated Carbohydrate Antigens — ***Sam Schmidt***, *Joelle Eaves, Theodore Belecciu, Nathaniel Pascual, Athar Nakissa, Shivangi Chugh, Xuefei Huang, Daniel Woldring*

4:42 Paper 21e: Engineering and Design of Tissue Inhibitor of Metalliproteinase-3 for Developing Protein Therapeutics — *Linh Do,* ***Maryam Raeeszadeh Sarmazdeh***

5:00 Paper 21f: Designing Hyperglycosylated Hemagglutinin Immunogens for Epitope-Focused Influenza Vaccines — ***Dana Thornlow***, *Aaron Schmidt*

5:18 Paper 21g: Simplifying Complex Antibody Engineering Using Machine Learning — ***Peter M. Tessier***

(22) Microbiome and Natural Products in Food, Health, and Bioprocessing

Sunday, Nov 13, 3:30 PM
Phoenix Convention Center, N-126C

Eirini Velliou, Chair
Shang-Tian Yang, Co-Chair

Sponsored by: Food

3:30 Paper 22a: Inducible Directed Evolution of an Anticancer Terpene Biosynthetic Pathway in *E. coli* — ***Zidan Li***, *Catherine Odhiambo, Ibrahim Al'Abri, Gavin Williams, Nathan Crook*

3:48 Paper 22b: Cas12a-Assisted Precise Targeted Cloning Using In Vivo Cre-*Lox* Recombination — ***Behnam Enghiad***, *Chunshuai Huang, Fang Guo, Guangde Jiang, Bin Wang, Huimin Zhao*

4:06 Paper 22c: The Role of Sigb on the (stress) Response of the Pathogen *Listeria Monocytogenes* to Novel Sustainable Processing Technologies. — ***Melina Kitsiou***, *Lisa Purk, Jorge Gutierrez-Merino, Kimon-Andreas Karatzas, Oleksiy Klymenko, Eirini Velliou*

4:24 Paper 22d: Characterization of Microbial Interactions in Stressed Environments for Construction of Synthetic Communities — ***Bradley Biggs***, *Markus de Raad, Trent Northen, Adam P. Arkin*

4:42 Paper 22e: Screening the Rhizobiome for Plant Growth Promoting Bacteria That Improve Maize Growth and Development — ***Ryan Hansen***, *Niloy Barua, Kayla Clouse, Maggie Wagner, Thomas Platt*

5:00 Paper 22f: Tools & Methods for Engineering Colonization of Plant Microbiomes — ***John Van Schaik***, *Akansha Pandey, Nathan Crook*

5:18 Paper 22g: [Keynote] Engineering Bacteria from the Plant Root Microbiome to Explore and Manipulate Plant-Microbe Interactions — ***Jonathan M. Conway***

(23) Systems and Quantitative Biology: Integrative Omics Analysis

Sunday, Nov 13, 3:30 PM
Phoenix Convention Center, N-125B

Rajib Saha, Chair
Christopher Kieslich, Co-Chair

Sponsored by: Bioengineering

3:30: Break

3:48 Paper 23b: Evaluating Proteome Allocation of *Saccharomyces Cerevisiae* Phenotypes with Resource Balance Analysis — ***Hoang Dinh***, *Costas D. Maranas*

4:06 Paper 23c: Metabolomics and Isotope Tracing Reveal the Dynamic Role of Parallel Glycolytic Pathways — ***Richard Law***, *Junyoung Park*

4:24 Paper 23d: Investigating the Neurodevelopmental Exposome: A Proposed Transcriptomic and Metabolomic Analysis of Mother-Child Cohort Pairs in Portugal — ***Dayna Schultz***, *Nafsika Papaioannou, Thanasis Papageorgiou, Aikaterini Gabriel, Ilias Frydas, Spyros Karakitsios, Dimosthenis Sarigiannis*

4:42 Paper 23e: Multi-Omics Approaches to Decipher Human Melanoma Initiation — ***Vivek Bajpai, MD, PhD***, *Tomek Swigut, Joanna Wysocka*

5:00 Paper 23f: Comparative Genomics and Phenomics Reveal Genetic and Functional Diversity and Fitness within *Pseudomonas Aeruginosa* clinical Isolates — ***Mohammad Mazharul Islam***, *Glynis Kolling, Jason A. Papin*

5:18 Paper 23g: Multi-Omics Integrative Analysis Using Mutual Information-Based Machine Learning — *Yan Tang*, ***Mark P. Styczynski***

(24) Value-Added Uses of Industrial Coproducts and Natural Fibres in Sustainable Uses

Sunday, Nov 13, 3:30 PM
Phoenix Convention Center, N-228A

Amar K. Mohanty, Chair
Manjusri Misra, Co-Chair

Sponsored by: Forest and Plant Bioproducts Division

3:30 Paper 24a: Chemical Pre-Lithiation of Lignin-Derived Hard Carbon Aimed for Lithium-Ion Battery Anode with High Rate Performance — ***Ruiqing Zhang***, *Xiaodong Hou, Xin Zhang, Yun Ji*

3:55 Paper 24b: Sustainable Biocomposites from Walnut Shell Powder Filled Poly(Butylene Succinate-co-Butylene Adipate) (PBSA)/Poly(Butylene Adipate-co-Terephthalate) (PBAT) Blend — ***Dayna McNeill***, ***Akhilesh Pal***, *Amar K. Mohanty, Manjusri Misra*

4:20 Paper 24c: Polybutylene Adipate Terephthalate-Based Biodegradable Composite Films: Effect of Talc Types on Mechanical and Water Vapor Barrier Properties — ***Shiv Shankar***, *Amar K. Mohanty, Manjusri Misra*

4:45 Paper 24d: Biodegradable Plastic Blends and Modified Starch-Based Sustainable Composite Films for Packaging Applications — ***Akhilesh Pal***, *Amar K. Mohanty, Manjusri Misra*

5:10 Paper 24e: Ethanol-Water Solutions at Elevated Temperatures for Isolating Ultraclean Corn Stover Lignins — ***Bronson Lynn***, *Graham W. Tindall, Villő E. Bécsy-Jakab, David Hodge, Mark C. Thies*

5:35 Paper 24f: Reactive Compatibilization of Biodegradable Blends from Phbv and Pbsa: Study on Effect of Chain Extender on the Mechanical, Thermal and Morphological Properties — ***Patricia Feijoo***, *Amar K. Mohanty, Arturo Rodriguez-Uribe, José Gámez-Pérez, Luis Cabedo,* ***Manjusri Misra***

(25) Advances in Biofuels Production and Alternative Fuels I

Sunday, Nov 13, 3:30 PM
Phoenix Convention Center, W-103A

Karthikeyan Ramasamy, Chair
Wang Shu, Co-Chair

Sponsored by: Fuels and Petrochemicals Division

3:30 Paper 25a: Thermocatalytic Conversion of Ethanol – a Pathway to Sustainable Aviation Fuel — ***Udishnu Sanyal***, *Mond F. Guo, Casper O. Brady, Senthil Subramaniam, Karthikeyan Ramasamy*

3:48 Paper 25b: Advancement of Catalytic Fast Pyrolysis of Biomass to Produce Renewable Fuels — ***Calvin Mukarakate***, *Kristiina Iisa, Huamin Wang, Daniel Santosa, Abhijit Dutta, Joshua Schaidle, Michael B. Griffin*

4:06 Paper 25c: Production of Renewable Diesel and Jet Fuel from Thermal Deoxygenation (TDO) Oil — ***Sampath Karunarathne***, ***Matthew J. Kline***, *Thomas Schwartz, Clayton Wheeler, Hemant P. Pendse*

4:24 Paper 25d: Accuracy of Predictions Made By Machine Learned Models for Biocrude Yields Obtained from Hydrothermal Liquefaction of Organic Wastes — *Feng Cheng,* ***Elizabeth Belden***, *Wenjing Li, Muntasir Shabuddin, Randy Paffenroth, Michael T. Timko*

4:42 Paper 25e: HTL of Wet Wastes for Sustainable Aviation Fuel — ***Michael R. Thorson***, *Dylan Cronin, Daniel Santosa, Senthil Subramaniam, Andrew J. Schmidt, Karthikeyan Ramasamy, John Norton Jr., Xavi Fonoll Almansa*

5:00 Paper 25f: Catalytic Hydrothermal Liquefaction of Food Waste: Improving Product Properties and Increasing Process Economic Viability — ***Hengameh Bayat***, *Mostafa Dehghanizadeh, Andrea Loya Luján, Catherine Brewer*

5:18 Paper 25g: Continuous Hydrotreatment of Sewage Sludge and *Spirulina* Algae Biocrudes from Hydrothermal Liquefaction: Different Catalysts for Different Organic Contaminants — ***Muhammad Salman Haider**, Daniele Castello, Lasse Rosendahl*

5:36 Paper 25h: Successful Jet Engine Testing of on-Specification Aviation Biofuels from Continuous Hydroprocessing of Hydrothermal Liquefaction Biocrudes — ***Muhammad Salman Haider**, Daniele Castello, Lasse Rosendahl*

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(26) Science Communication Session

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-227A

Victoria Muir, Chair
Christine Parrish, Co-Chair
Cory Thomas, Co-Chair

Sponsored by: Young Professionals Committee (YPC)

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(27) Biomaterials and Life Sciences Eng: Faculty Candidates I

Sunday, Nov 13, 3:30 PM
Phoenix Convention Center, N-122B

Ryan Koppes, Chair
Jouha Min, Co-Chair
Kelly Burke, Co-Chair
Jorge Almodovar, Co-Chair

Sponsored by: Biomaterials

3:30 Paper 27a: Competition of Folding-Induced Assembly and Liquid-Liquid Phase Separation Produces Diverse Morphologies of Homochiral Peptide Mixtures — ***Nairiti Sinha**, Craig J. Hawker, Matthew Helgeson*

3:48: Break

4:06 Paper 27c: Thermodynamic Control of Activity Patterns in Cytoskeletal Networks — ***Yuqing Qiu**, Alexandra Lamtyugina, Aaron Dinner, Suriyanarayanan Vaikuntanathan, Étienne Fodor*

4:24 Paper 27d: Label-Free Optical Recording of Bioelectrical Signals Harnessing Bio-Electrochromic Materials Interface — ***Yuecheng Peter Zhou***

4:42 Paper 27e: Self-Assembling Coatings to Protect Microbes from Processing Stressors — ***Gang Fan**, Ariel Furst*

5:00 Paper 27f: Bioresorbable Materials for Transient Batteries and Electrochemical Medical Devices — ***Yamin Zhang**, John A. Rogers*

5:18 Paper 27g: Biomaterial Strategies for Modulation of the Innate Immune System for Disease Amelioration — ***Apoorv Shanker**, Paula T. Hammond*

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(28) Biomaterials I: Biomaterials for Infection, Wound, and/or Disease Treatment

Sunday, Nov 13, 3:30 PM
Phoenix Convention Center, N-121A

Bethany Almeida, Chair
Xiaoping Bao, Co-Chair
Leah Spangler, Co-Chair
Murat Guvendiren, Co-Chair

Sponsored by: Biomaterials

3:30 Paper 28a: Controlling the Adhesive Behavior of Pathogenic Microorganisms on Polymeric Biomaterials — *Brandon Barajas, Meng-Chen Chiang, **Jessica Schiffman***

4:06 Paper 28b: A Cascade Nanozyme with Antimicrobial Effects against Otitis Media Pathogen — ***Xiaojing Ma**, Jiayan Lang, Pengyu Chen, Rong Yang*

4:24 Paper 28c: Understanding the Mechanism of Daptomycin Removal from the Gastrointestinal Tract Using Ion Exchange Biomaterials — ***Shang-Lin Yeh**, Amir Sheikhi, Landon vom Steeg, Robert Woods, Harrison Cassady, Sung Hyun Cho, Michael Hickner, Andrew Read*

4:42 Paper 28d: Kinetics and Thermodynamics of Peptide Binding and Peptide Release from Oxyntomodulin and Aib2-Oxyntomodulin Nano-Fibrils — ***Alireza Mohammad Karim**, Mark E. Welland, Ana L. Gomes Dos Santos*

5:00 Paper 28e: Light-Activated Skin Sealants for Rapid Wound Edge Approximation — ***Shubham Pallod**, Deepanjan Ghosh, Russell Urie, Jordan Yaron, Michelle McBride, Shelley Haydel, David DiCaudo, Jacquelyn Kilbourne, Kaushal Rege*

5:18 Paper 28f: Formulation Design and Coacervation of a Recombinant Protein-Based Lung Sealant — ***Jessica Torres**, Julie C. Liu*

5:36 Paper 28g: Novel Light Activated Biomaterial Based Films for Intestinal Tissue Sealing — ***Vanshika Singh**, Mallikarjun Gosangi, Deepanjan Ghosh, Kaushal Rege*

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(29) Biomaterials in Industry and the Clinic

Sunday, Nov 13, 3:30 PM
Phoenix Convention Center, N-121C

Eun Ji Chung, Chair
Forrest Kievit, Co-Chair
Runye Zha, Co-Chair
Julia E. Vela Ramirez, Co-Chair

Sponsored by: Biomaterials

3:30 Paper 29a: Keynote Speaker - Joseph Desimone, Professor of Translational Medicine and Chemical Engineering, Stanford University — ***Joseph M. DeSimone***

4:00 Paper 29b: Keynote Speaker - Amit Khandhar, Director of Formulations, HDT Bio — ***Amit Khandhar***

4:30 Paper 29c: Keynote Speaker - Omid Veiseh, Assistant Professor of Bioengineering, Rice University — ***Omid Veiseh***

5:00 Paper 29d: Combining Tunable Biomaterials and Flow-Based Membrane Technologies for Improved Biomanufacturing of T Cell Therapies — ***Kartik Bomb**, Paige LeValley, Ian Woodward, Zaining Yun, Bryan P. Sutherland, Samantha Cassel, Emily Kurdzo, Jacob McCoskey, Kara Levine, Christina Carbrello, Abraham Lenhoff, Catherine Fromen, April Kloxin*

5:15 Paper 29e: Stochastic and Deterministic Analysis of Reaction Kinetics in the Partially Reversible Copolymerization of Lactide and Glycolide — ***Louise Kuehster**, Feng Zhang, Nathaniel Lynd*

5:30 Paper 29f: Panel Discussion with Keynote Speakers — *Joseph M. DeSimone, Omid Veiseh, Amit Khandhar, **Runye Zha***

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(30) Charged and Ion Containing Polymers I

Sunday, Nov 13, 3:30 PM
Phoenix Convention Center, N-122A

Allie Obermeyer, Chair
Hee Jeung Oh, Co-Chair
Chibueze Amanchukwu, Co-Chair
Christian Aponte-Rivera, Co-Chair

Sponsored by: Polymers

3:30 Paper 30a: Polyelectrolyte Complex Hydrogels: A Platform for Wet Adhesives and 3D Bioprinting Inks — *Defu LI, Tobias Gockler, Ute Schepers, **Samanvaya Srivastava***

4:00 Paper 30b: Brushy Nanoparticle Complex Coacervates — ***Sarah Perry**, Mingjun Zhou, Maria M. Santore*

4:15 Paper 30c: Novel Crosslinked Ion Exchange Membranes with Phenyl Acrylate for Direct Urea Fuel Cell and Nonaqueous Flow Battery Applications — ***Jung Min Kim**, Yi-hung Lin, Yuyang Wang, Tina Huang, Jaesik Yoon, Sean Bannon, Charles Leroux, Patrick McCormack, Gary Koenig Jr., Geoffrey Geise, Dong-Joo Kim, Maria Auad, Bryan Beckingham*

4:30 Paper 30d: Investigation of the Doping Effects of Small Molecule Acids on Self-Healable, Stretchable PANI/Paampsa Conductive Polymer Complexes — ***Colton Duprey**, Hadi Rouhi, Nicole Penners, Katherine Webb, Elham Ghalavand, Sarah Veres, Gina Lusvardi, George Chen, Sofia Luna, Yang Lu, Ju-Won Jeon, Evan Wujcik*

4:45 Paper 30e: Electric Field Driven Transitions of Polyelectrolyte Complexes: From Spheres to Discoids to Prolate Ellipsoids — ***Aman Agrawal***, *Anusha Vonteddu, Matthew V. Tirrell, Jack F. Douglas, Alamgir Karim*

5:00 Paper 30f: Star Poly(ionic liquid)s — ***Kevin Nixon***, *Yossef Elabd*

5:15 Paper 30g: Water-Soluble Spiropyran Copolymers for Reversible Light-Induced Transition Metal Complexation and Removal — ***Harsheen Rajput***, *Chao Zeng, Boer Liu, James Brown, Lenore L. Dai, Timothy Long, Paul Westerhoff*

5:30 Paper 30h: Enhanced Proton Selectivity in Sulfonated Ionomer Nanocomposites Containing Fractionated, Clean Lignin — ***Xueting Wang***, *Mayura Silva, Bronson Lynn, Eric M. Davis, Stephen Creager, Mark C. Thies*

5:45 Paper 30i: Relationship between Ionic Conductivity and Polymer Properties in Electrolytes with Neutral Polymer Hosts: A Combined Simulation/Experimental Investigation. — ***Nathaniel Lynd***, *Venkat Ganesan, Sadahito Aoshima, Benny D. Freeman, Kazuya Maruyama, Jennifer Imbrogno, Frederick Rivers, Benjamin Pedretti, Congzhi Zhu, Jacob R. Baltzegar, Zidan Zhang, Paul W. Meyer*

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(31) Rising Stars in Industry – Polymers Research (Invited Talks)

Sunday, Nov 13, 3:30 PM
Phoenix Convention Center, N-121B

William Liechty, Chair
Mayank Misra, Co-Chair
Evan Wujcik, Co-Chair

Sponsored by: Polymers

3:30 Paper 31a: Building an Industrial Research Career in Polymer Science — ***Carla S. Thomas***

4:00 Paper 31b: Applying Polymer Material Science to Solve Problems in New Product Development — ***Praveen Agarwal***

4:30 Paper 31c: My Professional Development from Polymer Synthesis Chemist to Polymer Process Engineer — ***Pawel Krys***

5:00 Paper 31d: Applications of Fundamental Polymer Science to Increase the Performance and Efficiency of Polymeric Additives — ***Michael Petr***, *Owen Young, Jie Feng, Carlos Cruz, Paul Van Rheenen*

5:30 Paper 31e: Life after Graduate School: How Skillsets Learned in Academia Translate to Industry — ***Michelle Sing***

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(32) Applied Formulation Design in Drug Product

Sunday, Nov 13, 3:30 PM
Phoenix Convention Center, N-123

Brendon Ricart, Chair
Boung Wook Lee, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

3:30 Paper 32a: Tailored Composition of Lipid-Based Excipients for Improved Functionality in Advanced Pharmaceutical Manufacturing Processes — ***Sharareh Salar-Behzadi***, *Carolina Corzo, Moaaz Abdelhamid, MSc, Martin Spörk, Ana Belén Ocampo, Mira Maisriemler, Dirk Lochmann, Sebastian Reyer, Tanja Freichel*

3:51 Paper 32b: Formulation and Scale-up of Delamanid Nanoparticles for Oral Tuberculosis Treatment — ***Nicholas Caggiano***, *Joanna Georgiou, Madeleine Armstrong, Rodney Priestley, Robert K. Prud'homme*

4:12 Paper 32c: Preparation and Characterization of Modafinil Nanofibers By Electrospinning — ***Indumathi Sathisaran***, *Jean-Christophe Monbaliu, Cornelis Vlaar, Jorge Duconge, Vilmalí López-Mejías, Torsten Stelzer*

4:33 Paper 32d: Impact of Material Attributes and Process Parameters on Low Dose Powder Filling Using Drum Filler System — ***Tanu Mehta***, *Zhanjie Liu, Bruhal Shah, Justin P. Lacombe, Bodhisattwa Chaudhuri*

4:54 Paper 32e: Sepineo P600-Based Topical Semisolid Formulation- Relationship between Rheological Properties, Physical Stability, and Drug Release — ***Abu Zayed Md Badruddoza***, *Thean Yeoh, Dana Gates, Jaymin Shah*

5:15 Paper 32f: High Throughput Sterile Filtration of Highly Viscous Pharmaceutical Formulations — ***Mohannad Kadhum***, *Jack Kochevar, Ryan Swanson, Steve Laninga*

5:36 Paper 32g: Parameters for Controlling Liposome Particle Size By Extrusion — ***Maoqi Feng***, *Songqing Lu*

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(33) Predictive Scale-Up/Scale-Down for Production of Pharmaceuticals and Biopharmaceuticals I

Sunday, Nov 13, 3:30 PM
Phoenix Convention Center, N-122C

Onkar Manjrekar, Chair
Nicholas Vecchiarello, Co-Chair
Mary Eccles, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

3:30 Paper 33a: Synchronized Mixing, Bubble Size Distribution, and K_La High-Fidelity Simulation for Optimization, and Scale-up for Benchtop Biofilm Bioreactor — ***Jorge Lopez***, ***Nima Yazdanpanah***, *Ali Demirci, Aydin Berenjian*

3:52 Paper 33b: Process Development and Scale-up of an Enzyme Removal Strategy for Drug Substance Manufacturing — ***Victoria Zhang***, *Jonathan P. McMullen, Jungchul Kim, Kevin Sirk, Alexandra Sun, Daniel DiRocco, Joshua N. Kolev*

4:14 Paper 33c: Scale-Dependency Assessment Strategy to Translate Proven Acceptable Ranges from Small to Commercial Scale — ***Mary am Ende***, *Jacob Santos-Marques, David Am Ende, Matthew Burk, Fern Sinclair, Jerry S. Salan, David Leahy, Lopa Bakrania*

4:36 Paper 33d: Islatravir Crude Isolation Development and Scale-up: Late-Stage Shift from Filter Dryer to Centrifuge to Mitigate Risks from Enzyme Filtration — ***Brittany Dobson***, *Maggie Miller, Daniel Bishara, Matthew Gunsch, Michelle Cleary, David Bell, Aisling Prendergast, Ivan Lee, Darryl Chang, Sandra A. Robaire, Nicholas Rogus, Theodore Furman, Gregory Hughes, Elizabeth Fisher, Kevin Maloney, Junyong Jo, Paula Archbold*

4:58: Break

5:20 Paper 566c: *N-Glycanyzer*: An Integrated on-Line Process Analytical Toolkit for Enabling Continuous Biologic Manufacturing — *Aron Gyorgypal*, ***Shishir Chundawat***

5:42 Paper 33f: Antibody Production Against Camptothecin-Derived Small Molecules :a Tool for Developing Pharmacokinetic Studies and Dose Management Chemotherapy — ***Tahereh Zarnoosheh farahani***

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

Sunday, Nov 13, 3:30 PM
Phoenix Convention Center, N-224AB

Kishori Deshpande, Chair

Sponsored by: Product Design

3:30 Paper : Panel Discussion: Chemical Process and Product Design Careers in Industry & Academia — ***Kishori Deshpande***, ***Manjiri Moharir***, ***Grace Wan***, ***Lars Grabow***, ***Jindal Shah***

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(35) Process Intensification – Novel Technologies for Carbon Capture and Carbon Recycling

Sunday, Nov 13, 3:30 PM
Phoenix Convention Center, N-222A

David Lyons, Chair
Jonathan Lekse, Co-Chair

Sponsored by: Process Intensification & Microprocess Engineering

3:30 Paper 35a: Modeling CO_2 Capture in Liquid-Amine Infused Surfaces — ***Pedro Bertolini***, *Charles Maldarelli, Mohsen Yeganeh, Arben Jusufi, Shane Deighton*

3:51 Paper 35b: Rate-Based CO_2 Capture Modeling with Intrastage Cooling — ***Joshua Thompson***, *Gyoung Gug Jang, Costas Tsouris*

4:12 Paper 35c: Computational Fluid Dynamics (CFD) Modeling of Wetted Wall Absorption Columns for Solvent-Based Post-Combustion Carbon Capture Applications — ***Yash Girish Shah***, *Zachary Mills, Joshua Thompson, Debangsu Bhattacharyya, Costas Tsouris, Charles E. A. Finney,* ***Grigorios Panagakos***

4:33 Paper 35d: Three-Dimensional Computational Fluid Dynamics (CFD) Modeling of Post-Combustion Carbon Capture in Intensified Absorption Columns with Structured Packing. — ***Yash Girish Shah***, *Zachary Mills, Joshua Thompson, Debangsu Bhattacharyya, Costas Tsouris, Charles E. A. Finney,* ***Grigorios Panagakos***

4:54 Paper 35e: Improved Intra-Column Heat Removal from a CO_2-Capture Solvent System Via Modification of Additively Manufactured Intensified Packing Devices — ***Dhruba Jyoti Deka***, *Amiee Jackson, Gyoung Gug Jang, Joshua Thompson, Costas Tsouris*

5:15 Paper 35f: Production of Carbonates from Alkaline Industrial Waste Via Carbon Mineralization Towards a Circular Economy — ***Ning Zhang***, *Aaron Moment, Ah-Hyung Alissa Park*

5:36 Paper 35g: Energy-Effective Design of Steam Methane Reforming with Amine-Based CO_2 Capture and Storage (CCS) Process Using Liquefied Natural Gas Cold Energy — ***Hyeon-won Jeong***, *Khanh Vinh Nguyen, Shu Wang, Ricard Gutfraind, Ruichang Xiong, W. Jaewoo Shim*

(36) Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains I

Sunday, Nov 13, 3:30 PM
Phoenix Convention Center, N-226C

Radhakrishna Tumbalam Gooty, Chair
Dharik Mallapragada, Co-Chair
Edward Graham, Co-Chair

Sponsored by: Sustainable Energy

3:30: Break

3:45: Break

4:00 Paper 36c: Biomass, Solar and Wind-Based Hydrogen and Carbon Dioxide Supply Chain Optimization Considering Enhanced Oil Recovery: A Colombian Case Study — *Javier Oswaldo Lizcano Prada, Rafael Cristobal Garcia Saravia, Alexandra Duarte, Javier Angarita, Sandra Gómez, Leily Candela,* ***Ariel Uribe-Rodríguez***

4:15 Paper 36d: Assessing the Key Factors in the Transition to a Hydrogen-Based Economy through Agent-Based Simulation — ***Swaminathan Venkataramanan***, ***Rajagopalan Srinivasan***

4:30 Paper 36e: Co-Optimizing the Design and Operation Strategy of Solid Oxide Fuel Cell-Based Hydrogen-Electricity Co-Production Systems — ***Nicole Cortes***, *John C. Eslick, Alexander Noring, Naresh Susarla, Chinedu O. Okoli, Miguel A. Zamarripa, Arun Iyengar, Anthony P. Burgard, David Miller, Douglas A. Allan, Alexander Dowling*

4:45 Paper 36f: Natural Vs Engineering CO_2 Capture and Utilization — ***Guillermo Galán Iglesias Sr.***, *Mariano Martin, Ignacio Grossmann*

5:00 Paper 36g: Whole-System Value Chain Optimisation for Decarbonising Industrial Heat — ***Jennifer Penman***, *Sheila Samsatli*

(37) Reactor Engineering for Biomass Feedstocks

Sunday, Nov 13, 3:30 PM
Phoenix Convention Center, N-226B

Yukihiko Matsumura, Chair
Juan Restrépo-Florez, Co-Chair

Sponsored by: Sustainable Biorefineries

3:30 Paper 37a: Solid Fuel Formation By Co-Pyrolysis of Bamboo and Simulated Waste Plastic — ***Kenichiro Tanoue***, *Yuta Sasaki, Mai Kato*

3:45 Paper 37b: Flash Extractive Pyrolysis of Industrial Hemp Biomass to Produce Cannabidiol (CBD) — ***Foster Agblevor***, *Hamza Abdellaoui*

4:00 Paper 37c: Kinetic Studies on Pyrolysis of Invasive Reed Canary with a Combined Scheme of Parallel-Reaction Kinetic Model and Multi-Layer Artificial Neural Network Model — ***Hui Liu***, *Hesham Alhumade, Ali Elkamel*

4:15 Paper 37d: Detailed Gasification Process of Biomass-Derived Char and Gasification Mechanism — ***Md. Zakir Hossain***, *Naoki Matsu-ura,* ***Yukihiko Okumura***

4:30 Paper 37e: Ammonia Generation Rates for Hydrothermal Pretreatment of Chicken Manure — ***Yukihiko Matsumura***, *Yuito Suganuma, Takayuki Ichikawa, Wookyung Kim, Yutaka Nakashimada, Keiya Nishida*

4:45 Paper 37f: Production of Chemical Intermediates By Hydrolysis and Dehydration of Lignocellulosic B]Biomass Using Catalytic Membranes: Fundamental Research to Commercialization — ***Ranil Wickramasinghe***, *Xianghong Qian*

(38) 3D Printing Fundamentals and Applications

Sunday, Nov 13, 3:30 PM
Phoenix Convention Center, N-221B

Nese Orbey, Chair
Jung-Sheng Wu, Co-Chair
Lin Li, Co-Chair

Sponsored by: 3D Printing

3:30 Paper 38a: 3D printing all-aromatic polyimides with light: Photoreactive supramolecular polymeric salts as a versatile printing platform — ***Timothy E. Long***, *Christopher B. Williams*

4:10 Paper 38b: Commercialization of Additive Manufacturing, Some Pitfalls and Consideration — ***Nima Yazdanpanah***

4:50 Paper 38c: Digital Light Processing of Highly-Filled Polymer Composites with Tailorable Mechanical Properties — ***Amy Peterson***, *Ye Wang*

5:08 Paper 38d: Directionally Dependent Fluid Behavior from Uniform Periodic Structures: Influence of Design and Additive Process Parameters — ***Ian Woodward***, *Catherine Fromen*

5:26 Paper 38e: Understanding and Characterising the Spreading of Cohesive Powders in Powder Bed Fusion Additive Manufacturing Via Discrete Element Modelling — *Yi He, Ali Hassanpour,* ***Andrew Bayly***

5:44 Paper 38f: Improved Interlayer Adhesion in Fused Deposition Modeling (FDM) Printed Parts — ***Daniyal Shoukat***, *Jordan Totten, Jay Park, Nese Orbey, J Carson Meredith*

(39) Industry 4.0, Digital Twins, and Digital Transformation

Sunday, Nov 13, 3:30 PM
Phoenix Convention Center, N-221A

Masoud Soroush, Chair
Michael Baldea, Co-Chair

Sponsored by: Next-Gen Manufacturing

3:30 Paper 39a: Using Digital Technologies to Optimize Plant Uptime — ***Jonas Norinder***

4:00 Paper 39b: The Necessity of a Digital Toolbox — ***Wolter Last***

4:30 Paper 39c: Business Intelligence: A Case Study of a Chemical Plant — ***Abner Colman***, *Natalya A. B. Almeida, Fernanda Andrade, Heloyse Reges, Fernando V. Lima,* ***Heleno Bispo***

5:00 Paper 39d: Improving Control Room Operator Performance during Training Using a Cognitive Digital Twin — *Bharatwaajan B, Babji Srinivasan,* ***Rajagopalan Srinivasan***

5:30 Paper 39e: Investigating Model Predictive Control for a Wafer Etch Temperature Control System Using Computational Fluid Dynamics Simulations — *Henrique Oyama, Kip Nieman,* ***Helen Durand***

(40) 25th Anniversary of The Catalysis and Reaction Engineering Division I (Invited Talks)

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-129AB

Randall Meyer, Chair
Michael Harold, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

8:00 Paper 40a: The Catalysis and Reaction Engineering Division at 25 Years: Achieving the Vision — ***Michael Harold***

8:25 Paper 40b: Catalytic Chemical Reaction Engineering – Quo Vadis? — ***Jan Lerou***

8:50 Paper 40c: Alcohol Synthesis in a High-Pressure Membrane Contactor Reactor (MCR) Employing a Liquid Sweep — ***Jingwen Gong****, Fatemeh Sadat Zebarjad, Mohammad Bazmi, Linghao Zhao, Zhongtang Li, Kristian Jessen, Theodore Tsotsis*

9:15 Paper 40d: Thermo-Catalytic Versus Electro-Catalytic Hydrocarbon Activation: Enhancing Olefin Selectivity By Controlling the Oxide Ion Transfer — ***Umit Ozkan***

9:40 Paper 40e: Reactor Scale-up: Looking Forward By Looking Backward — ***Patrick Mills***

10:05 Paper 40f: Thermodynamic and Catalytic Properties of ALD-Grown Fe_2O_3 and $CeFeO_3$ Thin Films on High Surface Area Supports — *Kai Shen, Raymond J. Gorte,* ***John Vohs***

(41) Catalyst Design, Synthesis, and Characterization I: Dilute alloys

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-127C

Nathaniel Eagan, Chair
Casey O'Brien, Co-Chair

Sponsored by: Catalysis

8:00 Paper 41a: A Theoretical Framework for Rapid Screening of Novel Multi-Metallic Alloy Catalysts — ***Shikha Saini****, Joakim Halldin Stenlid, PhD, Frank Abild-Pedersen*

8:18 Paper 41b: Design of Single-Atom Alloys for Oxidation — ***Matthew Montemore***

8:36 Paper 41c: Reaction Driven Restructuring of PdCu Bimetallic Catalysts and Consequences for Selective Dehydrogenation and Oxidation Catalysis — *Zhaoru Zha, Georgios Giannakakis,* ***Prashant Deshlahra***

8:54 Paper 41d: Catalytic Effects of Metal Coordination in Dilute Bimetallic Alloy Nanoparticles — ***David Flaherty***

9:30 Paper 41e: Spectroscopic Probe Molecule Selection Using Quantum Theory, First-Principles Calculations, and Machine Learning — ***Joshua Lansford****, Dionisios Vlachos*

9:48 Paper 41f: Atom-By-Atom Mapping of the Electrocatalytic Activity of Multi-Metallic Nanoparticles — ***Saman Moniri****, Yao Yang, Jihan Zhou, Zipeng Zhao, Geng Sun, Colin Ophus, Yongsoo Yang, Ziyang Wei, Yakun Yuan, Cheng Zhu, Yang Liu, Qiang Sun, Qingying Jia, Hendrik Heinz, Jim Ciston, Peter Ercius, Philippe Sautet, Yu Huang, Jianwei Miao*

10:06 Paper 41g: Expanding Single-Atom Alloy Concept to Electrocatalysis: PGM Unexpectedly Facilitates Copper for Hydrocarbon Formations through CO_2 Reduction — ***Zehua Jin****, Manjeet Chhetri, John Yeager, Case Sandor, Hui Wang, Sungsik Lee, Cameron Bodenschatz, Ming Yang*

(42) Environmental Catalysis I: Applied Catalysis for Emissions Control

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-227B

Ming Yang, Chair
Eleni Kyriakidou, Co-Chair

Sponsored by: Catalysis

8:00 Paper 42a: CH_4 Conversion By Steam Reforming during Oxidation over Pt + Pd/Al_2O_3 Monolith Catalysts: Kinetic Model Development — ***Pak Wing Chen****, Kyle Karinshak, Ru-Fen Liu, Lars Grabow, Michael Harold*

8:20 Paper 42b: High-Silica Pd/H-LTA Catalysts for Low Temperature CH_4 Oxidation — ***Tala Mon****, Jingzhi Liu, Viktor Cybulskis, Eleni Kyriakidou*

8:40 Paper 42c: Fundamental Study of the Pretreatment Effect on the NiO_x/CeO_2 catalyst for NO+CO Reaction: Structure-Activity Relationship — ***Kyung-Min Lee****, Taejin Kim*

9:00 Paper 42e: Effect of Blending Hydrogen into Natural Gas on Selective Catalytic Reduction of NOx for Stationary Power Applications — ***Sahand Faraji****, Kyle Horiuchi, Bihter Padak*

9:20 Paper 42f: Effect of Water and CO on the NO_x Operating Cycle in Pd/CHA Passive NO_x Adsorbers — ***Marvi Kaushik****, Tuhin Suvra Khan, M. Ali Haider, Divesh Bhatia*

9:40 Paper 42g: Adsorbing & Oxidizing Abilities for Aromatic Species of Cu-Loaded BEA Zeolite As HC Trap during Cold Start Period — ***Jinseong Kim****, Eunhee Jang, Jungkyu Choi*

10:00: Break

(43) Fundamentals of Catalysis and Surface Science I: Hydrocarbon conversion chemistry

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-128B

Joaquin Resasco, Chair
Tibor Szilvasi, Co-Chair

Sponsored by: Catalysis

8:00 Paper 43a: First Principles Based Microkinetic Interrogation of Ethylene Oligomerization and Hydrogenation Potential of Transition Metal Ions Supported on Silica — ***Neha Mehra****, Nicole LiBretto, Guanghui Zhang, Jeffrey T. Miller, William Schneider*

8:20 Paper 43b: Demonstrating the Catalyst Reoxidation Mechanism: Alkene Dehydrogenation and Oxidation over VO_x/CeO_2 — ***Sol Ahn****, Justin Notestein*

8:40 Paper 43c: Propane Dehydrogenation on Different Pt Surfaces and Effect of Al_2O_3 Atomic Layer Deposition (ALD) — ***Hoan Nguyen****, Sumandeep Kaur, Liney Arnadottir*

9:00 Paper 43d: Kinetics and Pathways for the Catalytic Oxidation of Methane on $IrO_2(110)$ Thin Films — *Rachel Martin, Jovenal Jamir, Minkyu Kim, Christopher Lee, Vikram Mehar, Aravind Asthagiri,* ***Jason Weaver***

9:20 Paper 43e: Investigating the Genesis of Catalytic Promotion for Silica-Supported Molybdenum Oxide during Propylene Metathesis — ***Ran Zhu****, Husain Adamji, Zachariah Berkson, Jie Zhu, Ashley Head, Heather Kulik, Christophe Copéret, Yuriy Roman*

9:40 Paper 43f: First-Principles Design of Rh-Based Alloy Catalysts for Selective Propane Dehydrogenation — ***Seokhyun Choung****, Yoojin Lee, Hyeokjoon June, Heejae Yang, Jinuk Moon, Yoonho Kim, Yunkyung Kim, Kwang-Deog Jung, Jeong Woo Han*

(44) Microporous and Mesoporous Materials II: Material Design

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-128A

Viktor Cybulskis, Chair
James W. Harris, Co-Chair
Michele Sarazen, Co-Chair

Sponsored by: Catalysis

8:00 Paper 44a: La Incorporation in H-Mor Zeolite to Improve Shape Selectivity and Stability Against Coke Formation during the Alkylation of Toluene with Isopropanol — ***Nabihan Abdul Rahman***, *Daniel E. Resasco*

8:18 Paper 44b: Enhancing Zeolite-Based Catalysts Via Elemental Modification of Precursor States — ***Adam J. Mallette***, *Deependra Parmar, Jeffrey Rimer*

8:36 Paper 44c: Synthesis and Characterization of Zeolite-Encapsulated Organometallic Complexes for Oxidation Chemistries — ***Ethan P. Iaia***, *Jenna L. Groeber, Ambar Shrestha, Ganesh Rana, Amit Chowdhury, Charles Diemer, Martin G. Bakker, James W. Harris*

8:54 Paper 44d: Rational Design and Targeted Synthesis of Zeolites with the Assistance of Molecular Modeling, Structural Analysis, and Synthetic Chemistry — ***Dan Xie***

9:12 Paper 44e: Structure, Coordination, and Reactivity of Stable Ni-MIL-127 for Propylene Oligomerization with Active Sites Situated in the Framework — ***Benjamin Yeh***, *Saumil Chheda, Steven Prinslow, Adam Hoffman, Jiyun Hong, Jorge Perez-Aguilar, Simon Bare, Connie C. Lu, Laura Gagliardi, Aditya Bhan*

9:30 Paper 44f: Kinetic Investigation on the Solvation of Alkylamine Hofmann Elimination over Brønsted Acidic Zeolites — ***Han Chen***, *Omar Abdelrahman*

9:48 Paper 44g: Tuning Nanozeolite Hydrophobicity to Create Highly Active Catalysts for Alcohol Ring Opening of Epoxides — ***Nicholas Brunelli***, *Alexander Spanos, Leah Ford, Jee-Yee Chen*

10:06 Paper 44h: Interrogation of Alkaline Earth Ion Exchange and CO Vibrational Spectroscopy As Reporters of Al Proximity in CHA Zeolites — ***Wei Ge***, *Songhyun Lee, Sichi Li, Ahmad Moini, Subramanian Prasad, Anthony DeBellis, Rajamani Gounder, William Schneider*

(45) Multi-Scale Modeling

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-127B

Nitish Mittal, Chair
Joris Thybaut, Co-Chair
Jun Shi, Co-Chair

Sponsored by: Reaction Engineering

8:00: Break

8:18 Paper 45b: Accelerating the Scaleup Process for Complex Electrochemical Reactors Using a Smart Manufacturing Inspired Multiscale Modeling Approach — ***Derek Richard***, *Berkay Citmaci, Joonbaek Jang, Vito Canuso, Panagiotis Christofides, Carlos Morales-Guio*

8:36 Paper 45c: Multi-Scale Modelling of a Structured ZoneFlow^{TM} Reactor Coated with a Rh-Doped Ni Catalyst for Steam Methane Reforming — ***Minette Florent***, *He Zirui, Juray De Wilde*

8:54 Paper 45d: Kinetic Modeling of Catalytic Reduction of Carbon Dioxide to Methanol over Indium Oxide-Zirconium Oxide Catalyst — ***Jose Peter***, *Niket Kaisare, Jithin John Varghese*

9:12 Paper 45e: Bridging Simulations with Experiment: Predicting Solvent and Confinement Effects in Catalysis By Hydrophilic and Hydrophobic Zeolites — ***Alexander V. Mironenko***

9:30 Paper 45f: 3D-1D Modelling of Twin-Screw Extruders — ***Riccardo Togni***, *Christoph Kloss, Martin Lubej, Maximilian L. Eggersdorfer*

9:48 Paper 45g: A Multiscale Modeling Strategy for Monolith Reactors — ***Chaitanya Kavale***, *Niket Kaisare, Himanshu Goyal*

(46) Applications of Molecular Modeling to Study Interfacial Phenomena II

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-222B

Obioma Uche, Chair
Yamil Colón, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

8:00 Paper 46a: Characteristics of Droplet Explosions Studied with Non-Equilibrium Molecular Dynamics Simulations — ***Dominik Schaefer***, *Babette Kunstmann, Maximilian Kohns, Hans Hasse*

8:15 Paper 46b: Bubble Nucleation in the Surfactant Stabilized Polyol-CO_2 Mixtures:Insights from a Classical Density Function Theory Study — ***Sriteja Mantha***, *Huikuan Chao, Andrew Ylitalo, Benjamin Laccetti, Thomas Fitzgibbons, Weijun Zhou, Valeriy Ginzburg, Richard C. Flagan, Julia A. Kornfield, Zhen-Gang Wang*

8:30 Paper 46c: Interfacial Thermodynamics of Cryogenic Fluids: The Effect of Non-Condensable Gas on Fluid Storage — ***Michael DeLyser***, *Ashwin Ravichandran, Wayne J. Mullinax, John W. Lawson*

8:45 Paper 46d: Energy Optimization of Nanochannel Fluid Extraction with Various Channel Geometries — ***Zachary Diermyer***, *Yidong Xia, Jiaoyan Li*

9:00: Break

9:15 Paper 46f: Free-Energy of Monomeric Species in Uio-66 Metal-Organic Framework — ***Sanoj -***, *Yamil Colón*

9:30 Paper 46g: Structural Origin of Multiple Alkylated Cyclopentane As an Effective Lubricant — ***Jee-Ching Wang***, *Vidit Singh*

9:45 Paper 46h: Extracting Anisotropy Strength and Interfacial Free Energy of Al-Mg Alloy Under Rapidcooling Conditions Using Molecular Dynamics Simulations — ***Daniel Dolce***, *Pabitra Choudhury*

10:00 Paper 46i: Dynamic Evolution of Atomically Dispersed Catalysts — ***Nicholas Humphrey***, *Selin Bac, Shaama Mallikarjun Sharada*

10:15 Paper 46j: Molecular Simulations Study of Calcium Carbonate-Amino Acid-Dentin Interactions — ***Alina Emelianova***, *Max Maximov, Tatiana V. Brinzari, Andrei Potanin, Gennady Gor*

(47) Division Plenary: CAST (Invited Talks)

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-224AB

Alexander Mitsos, Chair
Martha Grover, Co-Chair

Sponsored by: Computing Systems and Technology Division

8:00 Paper 47a: In Memoriam of Babatunde a. Ogunnaike — ***Martha Grover***

8:05 Paper 47b: CAST Update — ***Martha Grover***

8:15 Paper 47c: CAST Programming Update — ***Alexander Mitsos***

8:20 Paper 47d: Identification of Sustainable Processes through an Integrated Process Synthesis Framework — ***Shuang Xu***, *Anjan K. Tula, Selen Cremaschi, Mario Eden*

8:45 Paper 47e: Optimization of an Air Separation Column Using a Complementarity-Based Vapor-Liquid Equilibrium Formulation — ***Vibhav Dabadghao***, *Jaffer Ghouse, Lorenz Biegler*

9:10 Paper 47f: Event Constrained Optimization — ***Joshua Pulsipher***, *Ignacio Grossmann, Carl Laird*

9:35 Paper 47g: Modeling the Progression of Fibrosis with Dysregulation of TGF-Beta in COVID19 Patients — *Mohammad Aminul Islam*, ***Ashlee Ford Versypt***

10:00 Paper 47h: AI-Based Hybrid Modelling for Chemicals-Based Product Design — *Rafiqul Gani*, ***Venkat Venkatasubramanian***

(48) Free Forum on Engineering Education: Junior and Senior Years

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, W-105A

Christi Luks, Chair
LiLu Funkenbusch, Co-Chair

Sponsored by: Undergraduate Education

8:00: Welcoming Remarks

8:02 Paper 48a: Teaching Fugacity through Comics and Assessing the Impact on Student Confidence and Understanding — ***Lucas Landherr***, *Francisco Hung, Rebecca L. Carrier*

8:20 Paper 48b: The Impact of an Optimization Mindset Focused on Long-Term Student Success: A Junior-Level Chemical Engineering Course Case Study — ***Kristen M. Wilding***, *Hayley Ford, Brad Bundy*

8:38 Paper 48c: Replacing Mimicry with Mastery: Homework Wrappers and Effort-Based Grading — ***Carl Lund***

8:56 Paper 48d: A Descriptive Study of a New Course on the History of Thermodynamics — ***Rachel Morrish***, *Eliza Buhrer*

9:14 Paper 48e: Enhancing Collaborative and Inclusive Skills Development to Foster Effective Chemical Engineering Capstone Design Teams — ***Courtney Pfluger***, ***Anastasia Hauser***, ***Sindia M. Rivera-Jimenez***

9:32 Paper 48f: An Approach to Addressing "Bio" Design within Capstone Design — ***Troy Vogel***, ***Mark J. McCready***

9:50 Paper 48g: Working with Industry in Rowan's Engineering Clinic Program — ***Jacob Martin***, *Erik Dunn, Emily Rooney, Andrew Sikora, Kirti Yenkie, C. Stewart Slater, Robert Hesketh*

10:08 Paper 48h: Using Mediawiki As an Online Collaborative Tool to Foster Learning in the Transport Phenomena Sequence at the University of South Florida — ***Ryan Toomey***

(49) Supporting Student Development of Professional Skills and Responsibilities

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, W-105B

Matthew Cooper, Chair
George Prpich, Co-Chair
Kristine Horvat, Co-Chair

Sponsored by: Education

8:00: Welcoming Remarks

8:02 Paper 49a: How We Incorporate the Impact of Engineering Solutions in Global, Economic, Environmental and Social Contexts — ***Taryn Bayles***, ***Joaquin Rodriguez Alonso***, ***Robert M. Enick***

8:20 Paper 49b: Incorporating the Stories of Scientific Discovery into the Chemical Engineering Curriculum. — ***Stephanie Velegol***

8:38 Paper 49c: Improving Scientific and Risk Public Communication of Process Safety Incidents for Chemical Engineering Undergraduates — ***Amanda Koh***, *Lance Simpson*

8:56 Paper 49d: Incorporating an Industry Role-Playing Experience in Laboratory Classes to Improve the Technical Communications of Students — ***Stephanie Wettstein***, *Jennifer Brown, Michelle Miley*

9:14 Paper 49e: Initial Offerings of an Undergraduate Research Methods Class: Results and Experiences — ***Joseph Holles***

9:32 Paper 49f: Professional Development for Students through Company Outreach — ***Jean Tom***, *Jennifer Lott, Mara Giga, Masano Huang*

9:50 Paper 49g: Coacheng: Virtual Mentoring for Chemical Engineering Students — ***Bryan Alamani***, *Jhud Mikhail Aberilla, Rowena Ordonez-Torres, Marjorie Baynosa*

10:08 Paper 49h: Study of Upper Division Chemical Engineering Students' Motivations in Selecting a First Position upon Graduation — ***Victoria Kolar***, *Allison Godwin*

(50) Unconscious Bias

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-226B

Eric Bell, Chair
Bryan Deschamps, Co-Chair

Sponsored by: Engineering for Inclusion

(51) Colloidal Dispersions

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-232A

Ubaldo M. Córdova-Figueroa, Chair
Javen Weston, Co-Chair

Sponsored by: Interfacial Phenomena

8:00 Paper 51a: Dynamic Interfaces for Multiscale Control of Colloidal Interactions — ***Yaxin Xu***, *Sho Takatori*

8:15 Paper 51b: Stability of Carbon Black Slurry Used in Flow Battery Applications — ***KangJin Lee***, *Mohan Das, Matthew Pitell, Christopher L. Wirth*

8:30 Paper 51c: Effect of a Double-Chain Surfactant on the Stabilization of Suspensions of Silica and Titania Particles Against Both Agglomeration and Sedimentation — *An-Hsuan Hsieh, Elias I. Franses,* ***David Corti***

8:45 Paper 51d: Diffusiophoresis Driven By Gradients of Macromolecules and Surfactant Systems — ***Angela Yang***, *Yingqi Yi, Aditya Khair, Stephen Garoff, Robert Tilton*

9:00 Paper 51e: Isolating Non-Gravitational Ageing Phenomena in Emulsions Utilizing Microgravity and Diffusing Wave Spectroscopy — ***Robert McMillin III***, *Valentina Lorusso, Marco Vaccari, Davide Orsi, Libero Liggieri, Luigi Cristofolini, James K. Ferri*

9:15 Paper 51f: Structural Dynamics and Kinetics of Rheological Aging of a Model Thermoreversible Colloidal Gel Following a Thermal Quench — ***Khushboo Suman***, *Norman J. Wagner*

9:30 Paper 51g: Brownian Dynamics Simulations of Shear-Induced Clustering of Electrostatically-Stabilized Colloidal Suspensions with Hydrodynamic Interactions — ***Marco Lattuada***

9:45 Paper 51h: Fantastic Gels and Where to Find Them: Toward Thermomechanical Processing of Colloidal Gels — ***Scott Fenton***, *Brian Ryu, Poornima Padmanabhan, Tuan T. D. Nguyen, Roseanna Zia, Matthew Helgeson*

10:00 Paper 51i: Inherent-State Melting and the Onset of Glassy Dynamics in Two-Dimensional Supercooled Liquids — ***Muhammad Hasyim***, *Dimitrios Fraggedakis, Kranthi K. Mandadapu*

(52) Electrochemical Advances to Enable Efficient Oxygen, Hydrogen and Water Reactions I

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-232C

Ian McCrum, Chair
Hui Xu, Co-Chair
Damilola Daramola, Co-Chair
Piran Kidambi, Co-Chair

Sponsored by: Electrochemical Fundamentals

8:00: Break

8:15 Paper 52b: Direct Seawater Electrolysis Enabled By Robust Ion Transport Control in Membrane Electrolyzers with Asymmetric Electrolyte Conditions — ***Joseph Perryman***, *Daniela Marin, Michaela Burke Stevens, Shannon W. Boettcher, Adam Nielander, Thomas Jaramillo*

8:30 Paper 52c: Theoretical Insight Toward Strain Tuning of Electrocatalysts for the Hydrogen Fuel Cell Applications — ***Zhenhua Zeng***, *Jeffrey Greeley*

8:45 Paper 52d: Modeling Hydrogen Evolution Reaction at the Buried Interface of Silica Coated Transition Metal Electrocatalysts from First Principles — ***Jianzhou Qu***, *Marissa Beatty, Daniel Esposito, Alexander Urban*

9:00 Paper 52e: Electricity + Air + Water = Hydrogen Peroxide — ***Haotian Wang***

9:15 Paper 52f: High Conductivity Hydroxide Conducting Membranes and Self-Adhesive Ionomers for Durable Alkaline Water Electrolysis and Fuel Cells — *Parin Shah, Habin Park, Dheeraj Nellithala,* ***Paul Kohl***

9:30 Paper 52g: Promoting the Volmer-Step Via Charge Transfer at the Interface of Pt/Carbon-Substrate Towards Efficient Alkaline Hydrogen Evolution — ***Lei Wang***

9:45 Paper 52h: Stability and Catalytic Activity of Non-Stoichiometric Overlayers in Bimetallic Systems — ***Trenton Wolter***, *Roberto Schimmenti, Vojislav Stamenkovic, Manos Mavrikakis*

10:00 Paper 52i: Influence of Alkali Metal Cations on the Hydrogen Evolution Reaction in Acidic and Basic Electrolytes — ***Jay Bender***, *Amanda Petersen, Frederik Cornelius Østergaard, Alexander Bagger, Mikayla Wood, Sean Heffernan, Jan Rossmeisl, Delia Milliron, Joaquin Resasco*

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(53) Faculty Candidates in CoMSEF/Area 1a, Session 1

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-222C

Amir Haji-Akbari, Chair
Jeremy Palmer, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

8:00 Paper 53a: Engulfment of Antifreeze Proteins By Ice — ***Aniket Thosar***, *Yusheng Cai, Sean Marks, Zachariah Vicars, Amish J. Patel*

8:12 Paper 53b: Fully Automated *in silico* Enzyme Engineering with a Simulation and Machine Learning Feedback Loop — ***Tucker Burgin***, *David Beck, Jim Pfaendtner*

8:24 Paper 53c: Hallucinating Native-like Antibodies with Deep Learning — ***Sai Pooja Mahajan***

8:36 Paper 53d: *Computational Design of Formulations and Biomaterials through Multiscale Modeling from All-Atom to Field-Theory* — ***Kevin Shen***, *My Nguyen, Nicholas Sherck, Stephan Kohler, Kris Delaney, M. Scott Shell, Glenn H. Fredrickson*

8:48 Paper 53e: Implicit Model Captures Electrostatic Features of Cell Membrane Environment — ***Rituparna Samanta***, *Jeffrey J. Gray*

9:00 Paper 53f: Building Deep Learning Architectures for Physics, Chemistry, and Biology with Geometric Algebra — ***Matthew Spellings***

9:12 Paper 53g: Thermodynamic Control of Organization and Self-Assembly of Cytoskeletal Networks Far Away from Equilibrium — ***Yuqing Qiu***

9:24 Paper 53h: Entropy Compartmentalization of Host-Guest Colloidal Clathrates — ***Sangmin Lee***, *Thi Vo, Sharon Glotzer*

9:36 Paper 53i: An Information-Driven Approach to Quantifying and Controlling Emergent Order — ***Ashley Guo***

9:48 Paper 53j: Digital Alchemy for the Inverse Design of Patchy Particles — ***Timothy C. Moore***, *Luis Y. Rivera-Rivera, Sharon C. Glotzer*

10:00 Paper 53k: Coarse-Grained Simulation of Self-Healing Supramolecular Polymers with Highly Branched Architectures — ***Cody Bezik***, *Amalie Frischknecht*

10:12 Paper 53l: Breakdown of the Stokes-Einstein Relation for a Passive Tracer in an Odd-Viscous Chiral Active Fluid — ***Anthony Poggioli***, *David Limmer*

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(54) Fundamentals of Interfacial Phenomena II

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-232B

Sepideh Razavi, Chair
Younjin Min, Co-Chair
Dongjin Seo, Co-Chair
Xiaoguang Wang, Co-Chair

Sponsored by: Interfacial Phenomena

8:00 Paper 54a: Interfacial Behavior and Droplet Interaction in Liquid-Liquid Systems — *Matthias Singer, Patrick Zimmermann,* ***Tim Zeiner***

8:15 Paper 54b: Modularizable Liquid Crystal-Based Open Surfaces Enable Programmable Chemical Transport and Feeding Using Liquid Droplets — ***Xiaoguang Wang***, *Yang Xu, Robert Dupont*

8:30 Paper 54c: Forced Wetting in a Square Capillary — ***Vignesh Thammanna Gurumurthy***, *Molly Baumhauer, Ilia Roisman, Stephen Garoff, Cameron Tropea*

8:45 Paper 54d: Interfacial Locomotion By Living Active Matter and Physical Analogs — ***Johnathan O'Neil***, *Victor Ortega-Jimenez, Xingwan Zhu, Prateek Sehgal, Hung-Tang Ko, M. Saad Bhamla*

9:00 Paper 54e: Marangoni Synergism in Binary Surfactant Mixtures — *Tsung-Lin Hsieh, Stephen Garoff,* ***Robert Tilton***

9:15 Paper 54f: Effects of Nanoparticles and Surfactants on the Interfacial Behavior of Oil and Water Under Nonequilibrium Conditions — ***Xuan Duy Thao Nguyen***, *Sepideh Razavi, Dimitrios Papavassiliou*

9:30 Paper 54g: Dynamic Adsorption and Pinching Dynamics of Polymer-Surfactant Complexes — ***Carina Martinez***, *Pulkit Saini, Chenxian Xu, Vivek Sharma*

9:45 Paper 54h: Drainage Via Stratification in Foam Films Made with Polymer-Surfactant Complexes — ***Chenxian Xu***, *Carina Martinez, Vivek Sharma*

10:00 Paper 54i: Salt Weakens Intermicellar Interactions and Structuring in Bulk and Foam Films — *Shang Gao, Chrystian Ochoa, Vivek Sharma,* ***Samanvaya Srivastava***

10:15 Paper 54j: Foam Film Drainage and Emulsification of Milk Proteins and Alternatives — *Lena Hassan, Chenxian Xu, Karim Al Zahabi, Nadia Nikolova, Michael Boehm, Stefan Baier,* ***Vivek Sharma***

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(55) Thermophysical Properties: Theory and Experiments for Charged Systems

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-223

Erik Santiso, Chair
Hiroyuki Matsuda, Co-Chair
Sanket Deshmukh, Co-Chair
Clare McCabe, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

8:00 Paper 55a: Beyond Flory-Huggins: Activity Coefficients from Perturbation Theory for Polar, Polarizable, and Associating Molecules from Solvents to Polymers — ***Walter Chapman***, *Wael A. Fouad*

8:20 Paper 55b: Electroneutrality Breakdown in Nanoconfined Domains — ***Pedro de Souza***, *Martin Z. Bazant*

8:40 Paper 55c: Effects of External Electric Fields on the Glass Transition of Ionic Liquids — ***Fernando J. Carmona Esteva***, *Yong Zhang, Yamil Colón, Edward Maginn*

9:00 Paper 55d: Phase Equilibria, Structural, and Dynamical Properties of so_2-binary Ionic Liquid Systems — ***Sudip Kumar Das***, *Reagan Black, Utkarsh Kapoor, Pratik Dhakal, Jindal Shah*

9:20 Paper 55e: Phase Equilibrium and Transport Properties of Water and Ionic Liquids Used in Biomass Processing — ***Karim Al-Barghouti***, *Abdul Butt, Abigail Haas, Aaron Scurto*

9:40 Paper 55f: Thermodynamic Properties of Aqueous Amino Acid Mixtures Using Coarse-Grained Molecular Dynamics Simulations — ***Marina Davidson***, *Kenneth Benjamin*

10:00 Paper 55g: Co-Oriented Fluid Functional Equation for Electrostatic Interactions (COFFEE) for Mixtures: Phase Behavior and Fluid Structure in Mixtures of Differently Polar Fluids — ***Joshua Marx***, *Maximilian Kohns, Kai Langenbach*

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(56) Advanced Treatment Technologies for Water

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-225A

Steven Weinman, Chair
Selma Mededovic, Co-Chair
Deepak Sharma, Co-Chair

Sponsored by: Water

8:00 Paper 56a: Photocatalytic ZnO Foams for Organic Micropollutant Degradation — ***Davide Mattia***

8:25 Paper 56b: Continuous Flow Catalytic Hydrogenation of Groundwater Nitrate in a Membrane Catalyst-Film Reactor — ***Juliana Levi***, *Hunter P. Jacobs, Chen Zhou, Michael S. Wong, Bruce Rittmann, Paul Westerhoff*

8:50 Paper 56c: Inducing Nanobubble Collapse Via Dynamic Stimuli to Generate ·OH for Contaminant Degradation — ***Gregg P. Kotchey***, *David V. P. Sanchez*

9:15 Paper 56d: Chemical-Free Water Treatment with Immobilized Dual-Porous Photocatalyst — ***Mary Worbington***, *Ella Sheets, Sam Snow, Kevin McPeak*

9:40 Paper 56e: Wastewater Treatment Using Anaerobic Membrane Bioreactors with Electrolytic Regeneration (AMBER) — ***Maryam Amouamouha***, *Travis Walker*

10:05 Paper 56f: Green Oxidation Processes for Industrial Wastewater Treatments — ***Kun-Lin Yang***

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(57) Atmospheric Chemistry and Physics: Modeling and Field Studies

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-225B

Marwa El-Sayed, Chair
Joseph Smith, Co-Chair

Sponsored by: Air

8:00 Paper 57a: The Breathing Human Infrastructure: Integrating Air Quality, Traffic, and Social Media Indicators — ***Marwa El-Sayed***, *Heather O'Leary, Scott Parr*

8:25 Paper 57b: Assessing Vehicle Contribution for CO and CO2 Emission in Los Angels Using BECO2N Sensor Network — ***Suverna Trivedi***

8:50 Paper 57c: Understanding the Performance of Low-Cost Sensors in Characterizing Particulate Matter (PM) in Outdoor and Indoor Environments — *Zahra Shivji,* ***Sabrina Westgate***, *Nga Lee Ng*

9:15 Paper 57d: Enhanced Light Absorption and Radiative Forcing By Black Carbon Agglomerates — ***Georgios Kelesidis***, *David Neubauer, Liang-Shih Fan, Ulrike Lohmann, Sotiris E. Pratsinis*

9:40 Paper 57e: Agent Based Approach for Prescriptive Mitigation of Exposure to Air Pollution in Urban Setting — ***Pranav Agrawal***, *Sathish Swaminathan, Raghunathan Rengaswamy*

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(58) Biomolecular Engineering II

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-126A

Xue Sherry Gao, Chair
Ashish Kulkarni, Co-Chair
Whitney Stoppel, Co-Chair
John Blazeck, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

8:00 Paper 58a: Development of a Plant Generated Therapeutic Made in-Flight to Treat Microgravity Osteopenia — ***Kevin Yates***, *Imran Khan, Yongao Xiong, Nancy E. Lane, Abhaya M. Dandekar, Karen A. McDonald, Somen Nandi*

8:18 Paper 58b: Self-Remodeling Protein Complexes Inspired By Fungal Cellulosomes — ***Stephen Lillington***, *M. Scott Shell, Michelle O'Malley*

8:36 Paper 58c: Use of Coiled-Coil Motifs to Assemble Membraneless Organelles for Tunable Control Liquid Liquid Phase Separation — ***Zhihui Su***, *Mikael Garabedian, Matthew C. Good, Daniel A. Hammer*

8:54 Paper 58d: Pro-Apoptotic Stapled Peptides Discovered Using Bacterial Cell Surface Display Demonstrate Improved Affinity, Specificity, and Efficacy — ***Marshall Case***, *Greg Thurber*

9:12 Paper 58e: *Lon* Deletion Impairs Persister Cell Resuscitation in *Escherichia coli* — ***Sayed Golam Mohiuddin***, *Aslan Massahi, Mehmet Orman*

9:30 Paper 58f: Investigating Bacterial Biofilm Infection in a 3D Bovine Airway Model — ***Neeti Gandhi***, *Padmavathy Rajagopalan*

9:48 Paper 58g: Invited Talk: Placeholder for the Invited Talk in the Biomolecular Engineering II Session — ***Whitney Stoppel***, *Xue Sherry Gao, John Blazeck*

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(59) Cell and Tissue Engineering: Engineering the Immune Response

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-126B

Laurel Hind, Chair
Panagiotis Mistriotis, Co-Chair
Whitney Stoppel, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

8:00 Paper 59a: Controlling the Immune Response through Controlling the Aggregation Kinetics of Engineered Peptides — *Gokhan Gunay, Seren Hamsici,* ***Handan Acar***

8:18 Paper 59b: Analysis of Microglia Morphology across Different Neuroinflammatory Rat Models — ***Hawley Helmbrecht***, *Elizabeth Nance, Kaleb Decker, Teng-Jui Lin, Sanjana Janakiraman, Mia Onodera*

8:36 Paper 59c: Regulation of Circadian Disruption through Inhibition of NOX2 in Microglia: A Potential Route to Target Neuroinflammation — ***Iswarya Muthukumarasamy***, *Jennifer M. Hurley, Jonathan S. Dordick*

8:54 Paper 59d: The Role of Myeloid Derived Suppressor Cells in the Immune Response to Infection — *Hannah Weppner,* ***Laurel Hind***

9:12 Paper 59e: Engineer CAR-Neutrophils from Hpscs for Targeted Cancer Immunotherapy — ***Xiaoping Bao***

9:30 Paper 59f: Temporal *ID2* transcription Factor Expression Improves Natural Killer Cell Differentiation from Human Pluripotent Stem Cells — ***Juhyung Jung***, *Yun Chang, Xiaoping Bao*

9:48 Paper 59g: Invited Talk: Placeholder for the Invited Talk for the Cell and Tissue Engineering: Engineering the Immune Response Session — ***Whitney Stoppel***, *Panagiotis Mistriotis, Laurel Hind*

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(60) Membrane and Process Technologies in Food and Bioprocess Engineering

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-131A

Xiaobin Jiang, Chair
Zishu Cao, Co-Chair

Sponsored by: Food

8:00: Delayed Start

8:18 Paper 60b: Porous Polytetrafluoroethylene Supported Silicalite Nanosheet Laminated Membrane Volatile Fatty Acid Separation from Anaerobic Bioreaction Broth — ***Zishu Cao***, *Landysh Iskhakova, Xinhui Sun, Maobing Tu, Junhang Dong*

8:36 Paper 60c: *Enhancing 'Dark' CO2 Fixation in Succinate Fermentations Via Hollow Fiber Membrane Carbonation and Strain Engineering* — ***Amanda Godar***, *Timothy Chase, Dalton Conway, Yen-Jung Lai, Bruce Rittmann, Xuan Wang, David Nielsen*

8:54 Paper 60d: Photo-Biocatalysis for Biomass Valorization — ***Jinguang Hu***, *Hamed Shirvani*

9:12: Break

9:30 Paper 60f: Science of Cutting Multi-Layer Systems: An Inspiration from Our Kitchens — ***Udita Ringania***, *Sunny Kumar, Tuhin Chakrabortty, M. Saad Bhamla*

9:48 Paper 60g: [Keynote] Recent Progresses in Particular Membrane Separation Techniques for Bioprocessing and Food — ***Kamalesh Sirkar***

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(61) New Methods in Protein Engineering

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-125A

James Van Deventer, Chair
Arnab Mukherjee, Co-Chair

Sponsored by: Bioengineering

8:00 Paper 61a: *In Vitro* Continuous Evolution of Proteins Via Bioautomata — ***Tianhao Yu***, *Haiyang Cui, Nilmani Singh, Huimin Zhao*

8:18 Paper 61b: Endoplasmic Reticulum Sequestration Empowers Phosphorylation Profiling on the Yeast Surface — *Jose Ezagui, Brittney Russell, Yave Mairena,* ***Lawrence A. Stern***

8:36 Paper 61c: Redesigning Known Proteins to Detect Insulin and IL-6 across a Four Order of Magnitude Concentration Range — ***Alan Richard****, Robert Pantazes*

8:54 Paper 61d: Correlating Protein Motor Structure with Function Via Novel Biophysical Approaches — ***Pushkar Lele***

9:12 Paper 61e: Engineering Dual Noncanonical Amino Acid Incorporation in Yeast — *Priyanka Lahiri,* ***James Van Deventer***

9:30 Paper 61f: Engineering Genetically-Encodable Oxygen-Independent Fluorescent Reporters Using Lov Proteins — ***Nolan Anderson****, Arnab Mukherjee*

9:48 Paper 61g: G-Protein Coupled Receptors: Protein Engineering Approaches to Improve Expression and Determine Protein-Protein Interactions — ***Anne Robinson***

(62) Systems and Quantitative Biology: Modeling Biological Processes

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-125B

Hyun-Seob Song, Chair
Siu Hung Joshua Chan, Co-Chair

Sponsored by: Bioengineering

8:00 Paper 62a: Predicting Antibody Titer Using Multi-Scale Dynamic Flux Balance Analysis Bioreactor Models — ***Saratram Gopalakrishnan****, Jasmine Tat, Miguel Angel Valderrama-Gomez, Fabrice Schlegel, William Johnson, Pablo A. Rolandi, Cleo Kontoravdi, Nathan Lewis*

8:18 Paper 62b: Characterizing the Interplay between Rubisco and Nitrogenase Enzymes of *Rhodopseudomonas Palustris* — *Rajib Saha, Adil Alsiyabi,* ***Niaz Chowdhury***

8:36 Paper 62c: Flux Balance Analysis at Single-Cell Level — ***Shriramprasad Venkatesan****,* ***Rudiyanto Gunawan***

8:54 Paper 62d: Nonlinear Modeling of the Estrogen Receptor Activity of Environmental Chemicals Using Classification Algorithms and Single-Cell Level Data — ***Zahir Aghayev****, Adam T. Szafran, Anh Tran, Hari S. Ganesh, Fabio Stossi, Lan Zhou, Michael A. Mancini, Efstratios N. Pistikopoulos, Burcu Beykal*

9:12 Paper 62e: Measurement and Modeling of Heterogeneous Single-Cell PI3K Inhibition Dose Responses — ***Patrick C. Kinnunen****, Gary D. Luker, Kathryn E. Luker, Jennifer J. Linderman*

9:30 Paper 62f: Nuclear Organization and Genome Regulation By RNA-Dependent Phase Separation — ***Krishna Shrinivas****, Jonathan E. Henninger, Ozgur Oksuz, Pradeep Natarajan, Phillip A. Sharp, Richard A. Young, Arup K. Chakraborty*

9:48 Paper 62g: Metabolic Modeling Tools in Kbase to Integrate Multi-Omics Data, Understand Microbiome Interactions, and Explore Energy Biosynthesis Mechanisms — ***Christopher S. Henry***

(63) Advances in Lignin Degradation Strategies

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-228A

Xianglan Bai, Chair
Sunkyu Park, Co-Chair

Sponsored by: Forest and Plant Bioproducts Division

8:00 Paper 63a: A Study for Kinetic Modeling and Experimental Validation of Lignin Fractionation with 4-Phenolsulfonic Acid for Effective Lignocellulosic Biomass Utilization — ***Juhyeon Kim****, Hyun-Kyu Choi, Anqi Ji, Mairui Zhang, Joseph Kwon, Chang Geun Yoo*

8:15 Paper 63b: Selective Oxidative Conversion of Acetylated Lignin Towards Aromatic Acids — ***Wenbo Peng****, Zhaohui Tong, Hanxi Bao, Dequan Xiao, Yigui Wang, William "Joe" Sagues, Helena Hagelin Weaver*

8:30 Paper 63c: Reaction Mechanism Determination for Fast Pyrolysis of a Model Lignin Tetramer Via Density Functional Theory — ***Ross Houston****, Nourredine Abdoulmoumine*

(64) Advances in Biofuels Production and Alternative Fuels II

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, W-103A

Karthikeyan Ramasamy, Chair
Wang Shu, Co-Chair

Sponsored by: Fuels and Petrochemicals Division

8:00 Paper 64a: Evaluation of Combustion Properties of Corn Stover-Derived Solid and Liquid Biofuels By Cone Calorimeter — ***Md Tahmid Islam****,* ***Jordan Klinger****, Toufiq Reza*

8:18 Paper 64b: Integrated Planning of Low-Iluc Biomass Production and Supply Chains for Advanced Biofuels: Towards the EU Biobased Economy — ***Dauda Ibrahim****, Sara Giarola, Calliope Panoutsou, Nilay Shah*

8:36 Paper 64c: Production of Sustainable Aviation Fuels from Lignocellulosic Biomass Feedstocks — ***Foster Agblevor****, Hossein Jahromi*

8:54 Paper 64d: Studies on the Optimization and Production of Bio-Ethanol from Cellulosic Material Using *Saccharomyces Cerevisiae* — ***Vishal Murali****, Arun Lanka, Anup Ashok, Bhanu Radhika Gidla*

9:12 Paper 64e: Evaluation of Ultra-High Temperature Resistant Preformed Particle Gels for Geothermal Preferential Fluid Flow Control — ***Tao Song****, Thomas Schuman, Baojun Bai*

9:30 Paper 64f: Roles of Urea Inclusion Fractionation of Biodiesel on the Cold Flow Properties and Establishment of Feedstocks for Biochemicals and Biomaterials — ***Junli Liu****, Bernard Tao*

9:48 Paper 64g: Novel Supercritical Biodiesel Plant Design and Process Scale-up — ***Shyam Paudel****,* ***Caleb Moellenhoff****, Haider Al-Rubaye, Joseph Smith*

10:06 Paper 64h: Development of Ni Supported Zeolite for Bio-Jet and Bio-Gasoline Fuels Production from Locally Grown Castor Seeds — *Masego Molefe,* ***Joshua Gorimbo****, Diakanua Nkazi*

(65) Developments in Electrochemical Reactors, Fuel Cells, and Electrolyzers I

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, W-102C

Jamelyn Holladay, Chair
Helen Lou, Co-Chair

Sponsored by: Fuels and Petrochemicals Division

8:00: Welcoming Remarks

8:05 Paper 65a: Carbon-Free Platinum Bismuth Alloy Nanoplatelets with Enhanced Activity and Platinum Stability in Operating Proton Exchange Membrane Fuel Cells and Electrolyzers — *Junchuan Fang, Pranjul Mani Dubey,* ***Anastasios Angelopoulos***

8:25 Paper 65b: Proton-Conducting Solid Oxide Electrolysis Cells Based on Doped-$BaZrO_3$ — ***Clarita Regalado Vera****, Hanping Ding, Jagoda M. Urban-Klaehn, Meng Zhou, Hongmei Luo, Dong Ding*

8:45 Paper 65c: Design and Development of a Kilowatt Scale Stack for Carbon Dioxide and Carbon Monoxide Electroreduction — ***Sean Overa****, Feng Jiao*

9:05 Paper 65d: Modelling the Electrochemical Reduction of CO_2 Under Gas-Liquid Taylor Flow — ***Isabell Bagemihl****, Chaitanya Bhatraju, J Ruud Van Ommen, Volkert van Steijn*

9:25 Paper 65e: Modular Dynamic Modeling of Electrochemical Reactors — ***Dominik Bongartz****, Luisa Carola Brée, Katharina Maria Ebeling, Matthias Leitl, Georgia Ioanna Prokopou, Jan Raphael Seidenberg, Alexander Mitsos*

9:45 Paper 65f: Tailoring Electrode Microstructures for High-Performance Redox Flow Batteries through Non-Solvent Induced Phase Separation — ***Charles Wan****, Rémy Jacquemond, Antoni Forner-Cuenca, Yet-Ming Chiang, Fikile R. Brushett*

10:05: Concluding Remarks

(66) Efficient Processing of Lignin to Bioproducts and Biofuels

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-228B

Bin Yang, Chair
Arthur Ragauskas, Co-Chair
Joshua Yuan, Co-Chair
Ning Sun, Co-Chair

Sponsored by: Green Process and Product Engineering

8:00 Paper 66a: Mechanism-Based Lignin Bioprocess and Biomaterial Design — *Qiang Li, Jorge Arreola Vargas, Cheng Hu, Furong Lin, Bin Yang, Arthur Ragauskas,* ***Joshua Yuan***

8:12 Paper 66b: Reductive Depolymerization of PAA-Fractionated Lignin Via Using Cupmo Catalyst — ***Anqi Ji****, Xianzhi Meng, Jingshun Zhuang, Jiseok Park, Kwang Ho Kim, Gyu Leem, Sung Bong Kang, Arthur Ragauskas, Chang Geun Yoo*

8:24 Paper 66c: Identifying Bacterial Lignin Degradation Pathways in *Pseudomonas Putida* KT2440 — *Zhangyang Xu,* ***Bin Yang***

8:36 Paper 66d: Production of Aromatics from Lignocellulosic Biomass: Vapor-Phase Hydrodeoxygenation of Propylguaiacol over a Bifunctional Molybdenum-Containing Zeolite — ***Jie Zhu****, Matthew Webber, Jamison Watson, Gregg T. Beckham, Yuriy Roman*

8:48 Paper 66e: Water-Based Wood Bio-Adhesive Made from Soy Protein Isolate and Depolymerized Lignin — ***Changle Jiang****, Jianli Hu*

9:00 Paper 66f: Valorization of Lignin: Continuous Fractionation Exploiting Sequential Precipitation — ***Arulselvan Ponnudurai****, Peter Schulze, Andreas Seidel-Morgenstern, Heike Lorenz*

9:12 Paper 66g: Monomers and Biocrude from Hydrothermal Liquefaction of Solvent-Fractionated Lignin — ***Ronish Shrestha****, Feng Cheng, Geoffrey Tompsett, Brent Scheidemantle, Charles M. Cai, Klaus Schmidt-Rohr, Michael T. Timko*

9:24 Paper 66h: Bioconversion of Rich Containing β-O-4 Linkage Lignin to Medium Chain Length-Polyhydroxyalkanoates — ***Jorge Arreola Vargas****, Bing Xu, Cheng Hu, Xianzhi Meng, Yun-Yan Wang, Arthur Ragauskas, Hugo Oscar Mendez-Acosta, Jose Antonio Perez-Pimienta, Joshua Yuan*

9:36 Paper 66i: Fractionation of Depolymerized Lignin Streams Using Tangential Flow Filtration — ***Dupeng Liu****, Asun Oka, Jipeng Yan, Ning Sun*

9:48 Paper 66j: Reductive Depolymerization of Lignin By Bifunctional Ru-Based Catalysts Supported on Tungstated-Zirconia — *Xiaojun Yang, Dequan Xiao,* ***Bin Yang****, Maoqi Feng*

10:00 Paper 66k: Lignin Bioconversion in a Unique Pelletized Cultivation Platform Using *Rhodococcus Opacus* PD630 Simplifies Biomass Harvesting and Enhances Lipid Production — *Bing Xu, Qiang Li, Yunqiao Pu, Shangxian Xie, Arthur Ragauskas,* ***Jorge Arreola Vargas****, Zhi-Hua Liu, Joshua Yuan*

(67) Fundamental Interactions of Microbes and Microbial Communities with Materials

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-222A

Tagbo Niepa, PhD, Co-Chair
Elizabeth Stewart, Co-Chair
Sricharani Balmuri, Co-Chair
Kunal Mondal, Co-Chair

Sponsored by: Miscellaneous

8:00 Paper 67a: Design Principles to Establish an Aerobic and Anaerobic Bacterial Community — ***Jenna Ott****, Catherine Day, Anna Hancock, Mohamed S. Abou Donia, Sujit Datta*

8:25 Paper 67b: Dynamic CRISPR-Based Genetic Programs in Microbe-Laden Hydrogels for Bioproduction — ***Widianti Sugianto****, Benjamin Tickman, Alshakim Nelson, James Carothers*

8:50 Paper 67c: Interaction of Micro- and Nano-Plastics with Marine Bacteria – What's Happening Under the Tip of the 'Plastic-Berg'? — ***Tania Silva de Oliveira****, Arijit Bose*

9:15 Paper 67d: The Histone H1-like Protein Algp Facilitates Even Spacing of Polyphosphate Granules in *Pseudomonas Aeruginosa* — ***Ravi Chawla****, Steven Klupt, Vadim Patsalo, Jamie Williamson, Lisa Racki*

9:40 Paper 67e: Adhesion Kinetics of *Staphylococcus Aureus* during the First Stages of Biofilm Evolution — ***Sarees Shaikh****, Patrick Ymele-leki*

(68) IACChE's James Y. Oldshue Lecture

Monday, Nov 14, 9:00 AM
Phoenix Convention Center, North Ballroom 120D

L. Antonio Estevez, Chair

Sponsored by: Liaison Functions

9:00: Introductory Remarks

9:15 Paper : Nanostructured Polymers for Energy Efficient Devices and Specialty Separation Applications — ***David Suleiman***

(69) Undergraduate Research Presentations - Chemicals, Biotechology, and Environment

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-231C

Cory Thomas, Chair

Sponsored by: Young Professionals Committee (YPC)

(70) Financial basics for Corporate decision-making

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, W-102B

Amanda Scalza, Chair
Elizabeth Haughton, Co-Chair

Sponsored by: Management Division

(71) Area Plenary: Leaders in Electronic and Photonic Materials (Invited Talks from Industry and Academia)

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-122B

Carissa Eisler, Chair

Sponsored by: Electronics and Photonics

8:00 Paper 71b: The Renaissance of Zinc|Manganese Dioxide Batteries: Revolutionizing the Landscape of Energy Storage Enabled Through Material Science Breakthroughs — ***Gautam Yadav***

8:45 Paper 71a: Manipulating the Optical and Dielectric Properties of Crystalline Thin Perovskite Films — *Thanh Le, Yin Yang, Samuel Johnson, Bryce Edmondson,* ***John Ekerdt***

9:30 Paper 71c: Synthesis and Novel Properties of Metal Halide Perovskites: From Quantum Dots to Magic Sized Clusters and Molecular Clusters — ***Jin Zhang***

(72) Biomaterials and Life Sciences Eng: Faculty Candidates II

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-121B

Ryan Koppes, Chair
Jouha Min, Co-Chair
Kelly Burke, Co-Chair
Jorge Almodovar, Co-Chair

Sponsored by: Biomaterials

8:00 Paper 72a: Immunomodulatory Biomaterials for Vaccines, Cancer, and Inflammation — ***Lisa Volpatti***

8:18 Paper 72b: The Effect of Heparin/Collagen Layer-By-Layer Coating in Immunomodulatory Functions of Mesenchymal Stromal/Stem Cells Stimulated By IFN-γ — ***Mahsa Haseli****, Jorge Almodovar*

8:36 Paper 72c: Design and Assembly of Biodegradable Engineered Micro- and Nanomaterials from Biopolymers — ***Muchun Liu***

8:54 Paper 72d: Hierarchical Control and Characterization of Biopolymer Materials — ***Gabriel Burks***, *Charles Schroeder*

9:12 Paper 72e: Comparing Uptake and Transport of Nanomaterials in Preclinical Blood Brain Barrier (BBB) Models Using a Layer-By-Layer Electrostatically Assembled Nanoparticle Library — ***Nicholas Lamson***, *Andrew Pickering, Jeffrey Wyckoff, Priya Ganesh, Joelle Straehla, Paula T. Hammond*

9:30 Paper 72f: High-Throughput Self-Assembly of Metal-Dipeptide Complexes into Tunable Chiral Structures — ***Prashant Kumar***, *Nicholas Kotov*

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(73) Biomaterials II: Biomaterials for Controlling Cell Behavior

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-122A

Bethany Almeida, Chair
Xiaoping Bao, Co-Chair
Leah Spangler, Co-Chair
Murat Guvendiren, Co-Chair

Sponsored by: Biomaterials

8:00 Paper 73a: Engineering Thermoresponsive Biomaterials for Investigating and Controlling Human Embryonic Stem Cell Function — ***David Schaffer***

8:36 Paper 73b: Temporal *ID2* transcription Factor Expression Improves Hpsc-Derived Natural Killer Cell Differentiation — ***Juhyung Jung***, *Yun Chang, Xiaoping Bao*

8:54 Paper 73c: Magnetized 3D Bioprinting to Fabricate Neural Assembloids — ***Lucia G. Brunel***, *Julien G. Roth, Michelle Huang, Sungchul Shin, Yueming Liu, Betty Cai, Sergiu P. Pasca, Sarah C. Heilshorn*

9:12 Paper 73d: Substrate Stiffness Regulates Microglial Phenotype and Function — ***Timothy Hackett***, *Srivatsan Kidambi*

9:30 Paper 73e: The Discontinuous Surface of Porous Membranes Can be Engineered to Reduce Cell-Substrate Interactions Similarly to Soft Materials — ***Thomas Gaborski***, *Zahra Allahyari*

9:48 Paper 73f: In-Vitro Assessment of the Biological Effects of Polymethyl Methacrylate in 2D and 3D Cellular Models — ***Luisa Barraza***, *Madeline Torres Lugo, Maribella Domenech, Wandaliz Torres García*

10:06 Paper 73g: Immunomodulatory Functions of Human Mesenchymal Stromal Cells Are Enhanced When Cultured on Hep/Col Multilayers Supplemented with Interferon-gamma — ***Mahsa Haseli***, *Jorge Almodovar*

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(74) Polymer Crystallization and Semi-Crystalline Polymers

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-121C

Jay Park, Chair
Kailong Jin, Co-Chair
Marat Andreev, Co-Chair

Sponsored by: Polymers

8:00 Paper 74a: Atomistic Simulation of Flow-Enhanced Nucleation and Flow-Induced Crystallization Above the Melting Point of Entangled Polymer Melts and Solutions Under Elongational Flow — ***Brian J. Edwards***, *Mohammad Hadi Nafar Sefiddashti, Bamin Khomami*

8:30 Paper 74b: Molecular Dynamics Simulation of Flow Enhanced Nucleation in Biaxial Flows — ***Chinmay Gangal***, *Gregory Rutledge*

8:45 Paper 74c: Molecular Dynamics Simulations of Composition-Dependent Crystal Nucleation in Polymer Blends — ***Wenlin Zhang***

9:00 Paper 74d: Acute Sensitivity of Polymer Crystallization Phase Behavior to Intermolecular Interactions — ***Pierre Kawak***, *Dakota S. Banks, Douglas Tree*

9:15 Paper 74e: Crystallization of Copolymers with Short-Chain Branching — ***Marat Andreev***, *Gregory Rutledge*

9:30 Paper 74f: Crystallization Kinetics and Thermal Modeling of Material Extrusion Additive Manufacturing of Two Polyamides — ***Amy Peterson***, *Masoumeh Pourali*

9:45 Paper 74g: Sensing the Melting Transition of Semicrystalline Polymers Via a Novel Fluorescence Technique — ***Richard Nile***, *Kailong Jin*

10:00: Break

10:15 Paper 74i: PEO Minority Block Crystallization in Asymmetric PEO-*B*-PCL Copolymers — ***Ryan Van Horn***, *Alex Ashley, Cole Tower*

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(75) Polymer Synthesis and Reaction Engineering

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-127A

Jimmy Lawrence, Chair
S. Eileen Seo, Co-Chair

Sponsored by: Polymers

8:00 Paper 75a: Synthesis of Ion Exchange Membranes for Large-Scale Energy Conversion and Storage Applications — ***Michael Hickner***

8:30 Paper 75i: Camphene as a Porogen for the Processing and 3D Printing of Porous Thermoplastics — ***Jeffrey Self***

8:45 Paper 75c: Cascade Ring Strain Release Polymerization of Cyclohexene Oxide Derivatives to Functional, High-Tg Polyethers Using a Mono(μ-alkoxo)Bis(alkylaluminum) Initiator — ***Benjamin Pedretti***, *Congzhi Zhu, Hironobu Watanabe, Sadahito Aoshima, Nathaniel Lynd*

9:00 Paper 75d: Precision Bottlebrush Polymers: Elucidating the Impact of Discrete Building Blocks — ***Nduka Ogbonna***, *Michael Dearman, Cheng-Ta Cho, Bhuvnesh Bharti, Andrew J. Peters, Jimmy Lawrence*

9:15 Paper 75e: Modular Synthesis of Functional Membranes: Boric Acid Removal from Wastewater — ***Frederick Rivers***, *Matthew Landsman, Benjamin Pedretti, Nathaniel Lynd, Benny D. Freeman, Lynn E. Katz, Desmond F. Lawler*

9:30 Paper 75f: Towards Miktoarm Polymers Via Sequence-Defined Oligocarbamate (SeDOC) Initiators — ***Adithya Rangamani***, *Christopher Alabi*

9:45 Paper 75g: Precision and Discrete Bottlebrush Polymers: Engineering Functions through Molecular Topology — ***Jimmy Lawrence***, *Nduka Ogbonna, Michael Dearman, Cheng-Ta Cho, Bhuvnesh Bharti, Andrew J. Peters*

10:00 Paper 75h: Designing Advanced Materials for Advanced Manufacturing: Striving for Sustainability — ***Timothy E. Long***, *Christopher B. Williams*

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(76) Nanoscale Science and Engineering Forum Division Plenary

Monday, Nov 14, 8:30 AM
Phoenix Convention Center, W-104B

Reginald Rogers Jr., Chair
Nigel Reuel, Co-Chair

Sponsored by: Nanoscale Science and Engineering Forum

8:30 Paper : NSEF Young Investigator Award - Research Acceleration in Nanoscience By Self-Driving Fluidic Labs — ***Milad Abolhasani***

9:20: Intermission

9:30 Paper : NSEF Forum Award - Nanomedicine: From High Tech to Global Health — ***Robert K. Prud'homme***

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(77) Division Plenary: In Memoriam — Dr. Douglas E. Leng (Invited Talks)

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-227C

Victor A. Atiemo-Obeng, Chair
Richard Calabrese, Co-Chair
Laura Dietsche, Co-Chair
De-Wei Yin, Co-Chair

Sponsored by: North American Mixing Forum

8:00 Paper 77a: In Memoriam — Dr. Douglas E. Leng: Opening Remarks — ***Richard Calabrese***

8:05 Paper 77b: Dr. Douglas E. Leng's Technical Contributions to the Dow Chemical Company and the NAMF Community — ***Laura Dietsche***, ***Victor A. Atiemo-Obeng***

8:30 Paper 77e: Progress on Mixing at Dow Inspired By Doug Leng — ***David West***

8:55 Paper 77c: Vision and Influence: Doug Leng's Focus on Computational Fluid Dynamics at the Dow Chemical Company — ***Joseph Smith***

9:20 Paper 77d: Emulsification and Dispersion in Agitated Liquid-Liquid Systems: Linking Hydrodynamics to Drop Size — ***Richard Calabrese***

9:45 Paper 77h: Tribute to Doug Leng By Cassian Lee

10:00 Paper 77i: Other Tributes to Doug Leng

10:10 Paper 77f: Remarks from the Leng Family — ***Ron B. Leng***

10:25 Paper 77g: In Memoriam — Dr. Douglas E. Leng: Closing Remarks — ***Suzanne Kresta***

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(78) Fluidization: Fundamentals

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, W-106C

Aaron Morris, Co-Chair
Michael Molnar, Co-Chair

Sponsored by: Fluidization and Fluid-Particle Systems

8:00 Paper 78a: An Analog of Rayleigh-Bénard Convection in Vibrated Gas-Fluidized Beds — *Qiang Guo, Yuxuan Zhang, Thomas M. Kovar, Kenan Xi,* ***Chris Boyce***

8:18 Paper 78b: Fluid-like Phenomena in Binary Granular Materials: Revealing the Physics behind Rising Granular Bubbles and Splitting Granular Droplets — ***Jens Metzger****, Ruben Strässle, Louis Girardin, Nicholas Conzelmann, Christopher McLaren, Christoph Müller*

8:36 Paper 78c: Role of Mass Loading on the Onset of Flow Modulation in a Dilute Turbulent Slurry in Eulerian-Lagrangian Simulations — *Mohamed Kasbaoui,* ***Jonathan Van Doren***

8:54 Paper 78d: Drag Reduction By Spherical Particles and the Role of Particle Clusters — ***Himanshu Dave****, Mohamed Kasbaoui*

9:12 Paper 78e: Maintaining Microstructure during Scaling in Circulating Fluidized Bed Risers — ***Ronald Breault***

9:30 Paper 78f: Assisted Fluidization of Cohesive Powders: X-Ray Tomography Analysis — ***Kaiqiao Wu****, Evert C. Wagner, Gabrie M.H. Meesters, J Ruud Van Ommen*

9:48 Paper 78g: Experimental Investigation of Flow Behavior and Segregation for Nonspherical Particles in the Multi-Component Mixture through a Fluidized Bed Solids Mixer. — ***Sanjay Kumar Verma****, Anshu Anand*

10:06 Paper 78h: Strategies for Engineering Two-Dimensional Nanomaterials for Efficient Water Transportation — ***Edison Ang***

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(79) Functional Nanoparticles and Nanocomposites

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, W-106A

Timothy Brenza, Chair

Sponsored by: Nanoparticles

8:00 Paper 79a: Thermomechanical Properties of Polyurea Nanocomposites over Extreme Strain Rates — ***Jessica Kopatz****, Elizabeth Jones, Brett Sanborn, Justin Wagner, Christopher Riley, Christine Cardinal Roberts*

8:15 Paper 79b: Light Extinction By Agglomerates of Gold Nanoparticles: A Plasmon Ruler for Sub-10 Nm Interparticle Distances — ***Georgios Kelesidis****, Daniel Gao, Fabian Starsich, Sotiris E. Pratsinis*

8:30 Paper 79c: Photothermal Conversion Efficiency of Multi-Color Emissive Carbon Dots: A Chemical and Thermal Analysis — ***Salar Balou****, Aashish Priye*

8:45 Paper 79d: *Probing Nanoparticle Interaction with Artificial Cell Membranes Via a High-Throughput Fluorescent Liposomal Leakage Assay* — ***Alison Lui****, Kranthi K. Mandadapu, Markita Landry*

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(80) Particulate Systems: Solids Handling, Processing, Conveying, Separation, and Heat Transfer

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, W-106B

Rohit Kumar, Chair
Yi Fan, Co-Chair

Sponsored by: Solids Flow, Handling and Processing

8:00 Paper 80a: Effect of Low Rotation Rate on Conduction and Radiation Heat Transfer in a Rotary Drum — ***Bhaumik Bheda****, Heather Emady*

8:18 Paper 80d: Comparative Study on the Collection Performance of a Coupled Cyclone with Built-in Circulating Granular Bed Filter for Geldart A and C Particles — ***Gao Sihong****, Yiping Fan, Chunxi Lu*

8:36 Paper 80e: Predicting the Effect of Particle Shape on Random Packing: The Case of Nonequant Shapes — ***Anna Jaeggi****, Anna-Maria Eckel, Ronny Pini, Ashwin Kumar Rajagopalan, Marco Mazzotti*

8:54 Paper 80f: Powder Electrostatics: Focus on Fundamentals Needed to Understand Applications — ***Geoffroy Lumay****, Eric Opsomer, Nicolas Preud'homme*

9:12 Paper 80g: Development of a Model for the Prediction of the Ignition Properties of Combustible Dusts Undergoing Homogeneous Combustion: Application to Sulfur Dust. — ***Jack Altwal****, Tomasz Olewski, Luc Vechot*

9:30 Paper 80h: The 20-L Chamber and the Provision of Dust Explosion Data for Industrial Use — ***Paul Amyotte***

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(81) Enabling Technologies: Drug Substance and Drug Product Manufacturing

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-123

Carla Luciani, Chair
Neil C. Dalvie, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

8:21 Paper 81c: Understanding of Heat Transfer in Freeze-Dryer during Primary and Secondary Drying Stages: Considerations of Vial's Thermal Properties — ***Kyu Yoon****, Vivek Narsimhan*

8:42 Paper 81d: Prediction of Tablet Dissolution from Real-Time Optical Coherence Tomography Data — ***Elisabeth Fink****, Stephan Sacher, Varun Kushwah, Maxwell Korang-Yeboah, Xin Feng, Huiquan Wu, Johannes G. Khinast*

9:03 Paper 81e: Imaging and Analysis of Lyophilized Structures By Micro-Computed Tomography — ***Isaac Wheeler****, Vivek Narsimhan, Alina Alexeenko*

9:24 Paper 81f: Minimal Purification of Recombinant Proteins for Early Developability Assessment — ***Sergio Rodriguez Aponte****, J. Christopher Love*

9:45 Paper 81g: In-Line Skin Thickness Evaluation on Co-Extruded Vaginal Rings By Means of Optical Coherence Tomography — *Matthias Wolfgang, Ioannis Koutsamanis,* ***Martin Spörk***

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(82) Predictive Scale-Up/Scale-Down for Production of Pharmaceuticals and Biopharmaceuticals II

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-122C

Onkar Manjrekar, Chair
Nicholas Vecchiarello, Co-Chair
Mary Eccles, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

8:00 Paper 82a: Implementation of a Small-Scale Capillary Shear Model to Facilitate Process Development of Disc Stack Centrifugation during the Harvest of Biopharmaceuticals — ***Steven Frey****, Jane Liao, Stijn H.S. Koshari, Robert Luo, Antonio Ubiera*

8:21 Paper 82b: Using Particle Size Distributions to Predict the Filterability of Materials throughout the Processing of Monoclonal Antibodies — ***Steven Frey****, Hong Zhang, Robert Luo, Antonio Ubiera*

8:42 Paper 82c: Predictive CFD Mixing Model for Scale up/Down of Large Molecule Dug Product Formulation — ***Matthew Flamm***, *Joseph Rizzo, Hope Seybold, Tracey Mascaro, Avik Sarkar, Shweta Modi, Chandler Amato, Craig Ikeda*

9:03 Paper 82d: Model Aided Scale-up of Spray Drying for a Sticky API (low Glass Transition Temperature) — ***Ankur Kapil***, *Li Liu, Claire Wombell, Michael Hamlin*

9:24 Paper 82e: In silico Modeling of Roller Compaction Processes for Scale-up and Tech Transfer: One Step Closer to Digital Twins — ***Elcin Icten Gencer***, *Dongying Shen, Duc Nguyen, David Perez-Aguilar, Mina Hamedi Rad, Shruti Gour, Saloni Daftardar, John Chung, Fernando Alvarez-Nunez, Fabrice Schlegel, Pablo A. Rolandi, Ananya Chowdhury, Maxwell Maritato, Rajarshi Sengupta, Killian Ryan*

9:45 Paper 82f: Optimizing the Design and Scale-up of Agitated Filter Dryer — ***Sravan Nallamothu***, *Guilherme Turezo, Mahesh Kadam,* ***Ahmad Haidari***

10:06 Paper 82g: Scalability and Predictability of Terminal Wet Milling Processes — ***Carla Luciani***, *Mary Eccles, Michael Filios*

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(83) Environmentally Friendly Product and Process Development for Sustainability

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-221C

Qiang Xu, Chair
Onkar Manjrekar, Co-Chair
Deboleena Chakraborty, Co-Chair

Sponsored by: Process Research and Innovation

8:00 Paper 83a: Enabling a Load-Flexible Operation of an Electrified Downstream Process for Bio-Based Carboxylic Acids — ***Christian Schröder***, *Marcel Gausmann, Andreas Jupke*

8:25 Paper 83b: Eco-Friendly Natural-Gas Monetization Complex for Simultaneous Productions of Power, Fertilizer, Methanol, and LNG with Inherent Carbon Capture — ***Ying Liu***, *Qiang Xu*

8:50 Paper 83c: Estimating Environmental Impacts at Early-Stage Process Synthesis Using Machine Learning Approach — ***Emmanuel Aboagye***, *C. Stewart Slater, Mariano J. Savelski, Robert Hesketh, Kirti Yenkie*

9:15 Paper 83d: Economic Analysis for Emission-Free Power Generation By Simultaneous Employing Fuel Sources of Natural Gas, Coal, and Biomass — ***Ying Liu***, *Vinaykumar Reddy Kothireddy, Qiang Xu*

9:40: Break

10:05 Paper 83f: Multi-Scale, Multi-Physics Modeling for the Design and Scale-up of a Novel Microchannel Cast Film Die — ***Laura Dietsche***, *Kurt Koppi, Daniel Ramirez, Jie Feng*

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(84) Regenerative Engineering Society I

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-121A

Nicholas Peppas, Chair
Karl Lewis, Co-Chair

Sponsored by: Regenerative Engineering Society

8:00: Regenerative Engineering Society Introduction, Cato T. Laurencin

8:20 Paper 84a: Regenerative Engineering: Enabling the Practice of Regenerative Medicine — ***Guillermo Ameer***

9:00 Paper 84b: Biomaterial Substrates to Promote Expansion and Function of Marrow Stromal Cells — ***Johnna S. Temenoff***

9:40 Paper 84c: Presentation Title Pending — ***Omolola Eniola-Adefeso***

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(85) Division Plenary: Gerhold and Kunesh Awards on Separations (Invited Talks)

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-124AB

Zunqing He, Chair
Anand Vennavelli, Co-Chair

Sponsored by: Separations Division

8:00 Paper 85a: Membrane Materials Under Complex Conditions — ***Zachary Smith***

8:30 Paper 85b: Tray Design, Operation, and Troubleshooting — ***Mark Pilling***

9:00 Paper 85c: Which Separation Method Needs Lower Power: Membrane or Distillation? — *Jose Adrian Chavez Velasco, Mohit Tawarmalani,* ***Rakesh Agrawal***

9:30 Paper 85d: Short History of Distillation with Trays — ***Daniel Summers***

10:00 Paper 85e: Na^+-Gated Nanochannel Membrane for Renewable Fuel Synthesis — ***Miao Yu***

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(86) Big Data and Analytics for Sustainability

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-226A

Raymond Smith, Chair
Vassilis Charitopoulos, Co-Chair

Sponsored by: Sustainability Science and Engineering

8:00 Paper 86a: A Data Mining Framework for Collecting Chemical-Centric Data for End-of-Life Flow Inventory — *Jose Hernandez-Betancur,* ***Gerardo Ruiz-Mercado***, *Mariano Martin*

8:25 Paper 86b: Development of Predictive Modeling Tool for Wastewater Asset Modeling and Management — ***Jake Stengel***, *Dylan Snyder, Natheniel Nelson, Emmanuel Aboagye, Matt DeNafo, Kirti Yenkie*

8:50 Paper 86c: Plant-Wide Digital Twinning of Surface Finishing for Sustainable Manufacturing — ***Abdurrafay Siddiqui***, *Mahboubeh Moghadasi, Yinlun Huang*

9:15: Break

9:40 Paper 86e: Application of Machine Learning-Based Approach in Synthesizing Optimal Ionic Liquids for CO_2 Capture — ***Sadah Mohammed***, *Kazi Khoda, Fadwa Eljack, Saad Al-Sobhi*

10:05 Paper 86f: Study on the Mechanism of Alcohol Ether System Separation By Ionic Liquids Based on Density Functional Theory — ***Yanli Zhang***

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(87) Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains II

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-226C

Radhakrishna Tumbalam Gooty, Chair
Edward Graham, Co-Chair
Dharik Mallapragada, Co-Chair

Sponsored by: Sustainable Energy

8:00 Paper 87a: Designing Green Corridors for Sustainable Maritime Transportation — ***Hanchu Wang***, *Prodromos Daoutidis, Qi Zhang*

8:21 Paper 87b: THESEUS: An Optimal Design and Downselection Framework for Energy Storage Technologies — *Manali S. Zantye,* ***Akhilesh Gandhi***, *Mengdi Li, Pavitra Senthamilselvan Sengalani, Yifan Wang, Sai Pushpitha Vudata, Debangsu Bhattacharyya, M M Faruque Hasan*

8:42 Paper 87c: Impact of Renewable Energy Sources Integration on Profit and CO_2 Emissions in Chemical Process Networks — ***Ioannis Giannikopoulos***, *Alkiviadis Skouteris, David Allen, Michael Baldea, Mark Stadtherr*

9:03 Paper 87g: Integrating Intensive Livestock and Cropping Systems: Sustainable Design and Location — ***Manuel Taifouris***, *Mariano Martin*

9:24 Paper 87e: Transforming the Chemicals and Materials Industry Toward Net-Zero Greenhouse Gas Emissions: Approach and Preliminary Results — ***Amrita Sen***, *Vyom Thakker, George Stephanopoulos, Bhavik Bakshi*

9:45 Paper 87f: Exploring the Role and Value of Bidirectional Electric Vehicle Dispatch in Low-Carbon Power Systems — ***James Owens***, *Ian Miller, Emre Gençer*

(88) Applications of Data Science to High Throughput Experimentation

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-230

Elizabeth Nance, Chair
Connor Coley, Co-Chair
Curtis Martin, Co-Chair

Sponsored by: Applications of Data Science to Molecules and Materials

8:00 Paper 88a: A Bayesian Experimental Design Framework for Optimizing Microbial Communities — ***Jaron Thompson***, *Ophelia Venturelli, Victor Zavala*

8:15 Paper 88b: Solution Coating of Polymer Blend Libraries for High-Throughput Experimentation Via Passive Mixing — ***Aaron L. Liu***, *Ezgi Melis Dogan-Guner, Michael McBride, Rahul Venkatesh, Miguel A. Gonzalez, Jun Amano, Elsa Reichmanis, Martha Grover, J Carson Meredith*

8:30: Break

8:45 Paper 88d: Design of an Automatic Platform for Machine-Learning Model Based Molecular Property Optimization — ***Matthew McDonald***, *Brent Koscher, Richard Canty, Seung Kyun Ha, Camille Bilodeau, Kevin P. Greenman, Charles J. McGill, Rafael Gomez-Bombarelli, William Green, Klavs Jensen*

9:00 Paper 88e: Simulating Closed-Loop Catalyst Discovery Processes Using an Experimental Band Gap Surrogate Model — ***Kirby Broderick***, *Zachary Ulissi*

9:15 Paper 88f: Improved Characterization of Membrane Transport Properties through Advanced Data Analytics — ***Xinhong Liu***, *Jonathan Ouimet, Laurianne Lair, William Phillip, Alexander Dowling*

9:30 Paper 88g: Autonomous Optimization of Robotic Process Parameters for Accurate Experiments — ***Martin Seifrid***

9:45 Paper 88h: High-Throughput Screening of Binary and Ternary Organic Redox Active Materials-Based Deep Eutectic Solvents — ***Maria Politi***, *Jaime Rodriguez Jr., Stuart Adler, David Beck, Lilo Pozzo*

(89) Medical Devices

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-126C

Bernard Van Wie, Chair
William Pitt, Co-Chair

Sponsored by: Chemical Engineers in Medicine

8:00 Paper 89a: Low-Level Metal Toxicology in Serum Via Anodic Stripping Voltammetry — ***Shaylee R. Larson***, ***Mary Jeppson***, *Kevin Chandler, Paige Leland, Himanshu Sant, Swomitra Mohanty*

8:21 Paper 89b: Comparison of Methemoglobin and Deoxyhemoglobin As Potential Contrast Agents in Magnetic Resonance Imaging (MRI) — ***Royaalsadat Ayati***, *Kyle Manwaring, Randy S. Lewis*

8:42 Paper 89c: Barrier-Free Paper Analytical Devices for Multiplex Colorimetric Detection — ***Ayushi Chauhan***, *Bhushan Toley*

9:03 Paper 89d: Clinical Validation of Breath Biomarkers in Pediatric Tuberculosis Patients Using Comprehensive Two-Dimensional Gas Chromatography Time-of-Flight Spectrometry — ***Mary Jeppson***, *Emily Lym, Swomitra Mohanty*

9:24 Paper 89e: Elucidating the Effects of Shear and Surface Topography on Thromboembolism in Ventricular Assist Devices — ***Anjana Jayaraman***, *Junhyuk Kang, James Antaki, Brian J. Kirby*

9:45 Paper 89f: Active Levy Swimmers and Geometric Design for Anti-Infection Catheters — ***Tingtao Zhou***

10:06 Paper 89g: A Low Cost, Compact Flow Cytometer — ***Mahrukh Mir***, *Mahesh S. Tirumkudulu*

(90) Entrepreneurship in Chemical Engineering (Invited Talks)

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, W-103B

Nese Orbey, Chair

Sponsored by: Entrepreneurship in Chemical Engineering

8:00 Paper 90a: Invited Presentation by Chett Boxley — ***Chett J. Boxley***

8:25 Paper 90b: Invited Presentation from Phillip Lacovara — ***Philip Lacovara***

(91) Applied Artificial Intelligence, Big Data, and Data Analytics Methods for Next-Gen Manufacturing Efficiency I

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-221A

Davood Babaei Pourkargar, Chair
Joel Paulson, Co-Chair

Sponsored by: Next-Gen Manufacturing

8:00 Paper 156b: Keynote Talk-Machine Learning Based Software Tool for Efficient Wastewater Asset Management — ***Kirti Yenkie***, *Jake Stengel, Emmanuel Aboagye, Matt DeNafo*

8:21 Paper 91b: Partially-Connected Recurrent Neural Network Modeling for Predictive Control Using Noisy Data — ***Mohammed Alhajeri***, *Zhe Wu, Panagiotis Christofides*

8:42 Paper 91c: Handling Correlated Data for Artificial Neural Network (ANN)-Based Model Predictive Control (MPC) Implementations — ***Hesam Hassanpour***, *Brandon Corbett, Prashant Mhaskar*

9:03 Paper 91d: Application of Data Driven Techniques to Industrial Hydroprocessing Units — ***Debanjan Ghosh***, *Jesus Moreira, Prashant Mhaskar*

9:24 Paper 91e: Investigating Machine Learning Techniques for Effective Predictive Maintenance in Industrial Systems — ***Mahdi Ahmed***, *Louis Allen, Joan Cordiner*

9:45 Paper 91f: Hallucinating Inexpensive, Diverse and Native-like Antibodies with Deep Learning — ***Sai Pooja Mahajan***

10:06 Paper 91g: Forecasting and Reconstructing Chaotic Dynamics from Partial Observable Data — ***Charles Young***, *Michael Graham*

(92) Sensors and Monitoring for Health

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, N-231A

Evan Wujcik, Chair
Gang Fan, Co-Chair

Sponsored by: Sensors for Sustainability

8:00 Paper 92a: Session Introduction — ***Evan Wujcik***, ***Gang Fan***

8:10 Paper 92b: Smart Bandage for Online Monitoring and Treatment of Infected Chronic Wounds — ***Ehsan Shirzaei Sani***, *Wei Gao*

8:30 Paper 92c: Fabric-Based Wearable Health Sensors — ***Chelsea Monty-Bromer***

8:50 Paper 92d: Dopamine Modified Carbon Fiber Micro-Electrodes for Enhanced Detection of Cu(II) Via Fast Scan Cyclic Voltammetry — *Noel Manring*, ***Muzammil Nishar Ahmed***, *Jonathan Xavier, Lexine Sibert, Pavithra Pathirathna*

9:10 Paper 92e: Highly Selective Biosensor Based on Ionic Liquids-Assisted Colorimetric Sensing for Arsenite — ***Sam Li***, *Xuan Hao Lin*

9:30 Paper 92f: Dynamic Measurement of Endogenous Acetone in Exhaled Breath As a Non-Invasive Alternative to Obtain Diffusing Capacity of the Lung — ***Anastasios Angelopoulos***, *Jonathan A. Bernstein*

(93) Powering the Future: Panel Discussion

Monday, Nov 14, 11:00 AM
Phoenix Convention Center, N-124AB

Sindee Simon, Co-Chair
De-Wei Yin, Co-Chair

Sponsored by: Keynotes and Plenaries

(94) 2022 Danckwerts Lecture

Monday, Nov 14, 11:15 AM
Phoenix Convention Center, North Ballroom 120D

Sankar Nair, Chair

Sponsored by: Awards Committee

11:15 Paper : Working with CO_2 — ***Diane. Hildebrandt***

(95) Angel Investing in Chemical Startups: Putting Your Experience to Work

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, W-103B

Mark Vreeke, Chair
William Byers, Co-Chair

Sponsored by: Entrepreneurship in Chemical Engineering

3:30: Introductory Remarks

3:35: Introduction to Angel Investing

3:50 Paper 95a: Angel Investing Panel Discussion — ***William Byers, Ryan C. Smith, Charla Triplett, David Youngentob, Hugh James***

4:40: Concluding Remarks

(96) 25th Anniversary of The Catalysis and Reaction Engineering Division II (Invited Talks)

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-129AB

Anne Gaffney, Chair
Concetta La Marca, Co-Chair
Randall Meyer, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

12:30 Paper 96a: Reflections on 25 Years in the CRE Division and Hydrothermal Reaction Engineering — ***Phillip E. Savage***

12:55 Paper 96b: Developing Strategies for Polymer Redesign and Recycling Using Reaction Pathway Analysis — ***Linda Broadbelt***

1:20 Paper 96c: Thermochemical Conversion of Waste Biomass — ***Susan Stagg-Williams***, *Joao Poli, Mary Sevart, Sara Schafer*

1:45 Paper 96d: Sharing Good Times with Friends in the CRE Division: Past, Present and Future — ***John Kitchin***

2:10 Paper 96e: The Challenges of Energy Transition — ***Fabio H. Ribeiro***

2:35 Paper 96f: How CRE Has Shaped and Continues to Revolutionize the Multi-Trillion Dollar Energy and Petrochemicals Industry. — *Sarika Goel,* ***Kurt VandenBussche***

(97) Catalysis in Liquid Media I: Catalysis for Biomass Conversion in Liquid Phase

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-127B

Nirala Singh, Chair
Neeraj Rai, Co-Chair

Sponsored by: Catalysis

12:30 Paper 97a: Adsorption Free Energy Surfaces of Lignin Dimers over Zeolite Nanosheets in Solution — ***Woodrow Wilson***, *Neeraj Rai*

12:50 Paper 97b: Investigating Reaction Mechanisms and Solvent Effects in Humins Formation Using Multiscale Molecular Modeling — *Samir H. Mushrif,* ***José Carlos Velasco Calderon***, *Jyotsna S. Arora*

1:10 Paper 97c: Tuning the Reactivity of Hydrogen Species at Solvent-Metal Interfaces for the Activation of Strong Polar Bonds: Hydrodeoxygenation of Phenolics — ***Alyssa Hensley***, *Junnan Shangguan, Haoyu Nie, Ya-Huei (Cathy) Chin, Jean-Sabin McEwen*

1:50 Paper 97d: Activity of Pt_xCo_y Alloys for Phenol Hydrogenation in the Aqueous Phase — ***James Akinola***, *Isaiah Barth, Takaaki Miki, Bryan Goldsmith, Nirala Singh*

2:10: Break

2:35 Paper 97f: Confinement Effects on Solvation Thermodynamics of Biomass Adsorbates in Zeolites — ***Xiuting Chen***, *Rachel Getman*

(98) Catalyst Design, Synthesis, and Characterization II: Dynamics and stability

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-127C

Matteo Cargnello, Chair
Tae-Sik Oh, Co-Chair

Sponsored by: Catalysis

12:30 Paper 98a: Templated Encapsulation of Pt-Based Catalysts Promotes High-Temperature Stability to 1,100 °C — ***Aisulu Aitbekova***, *Simon Bare, Matteo Cargnello*

12:48 Paper 98b: Understanding the Criteria for Controlling Catalyst Restructuring and Redispersion — ***Alexander Hill***, *Galen Fisher, Andrej Lenert, Johannes Schwank*

1:06 Paper 98c: Dynamics of Exsolved Ni-Fe Catalysts in Redox Environments — *Soham Shah, Jiyun Hong, Luz Cruz, Simon Bare,* ***Kandis Leslie Abdul-Aziz***

1:24 Paper 98d: Characterizing Dynamic Materials for Electrocatalytic Processes — ***Linsey Seitz***

2:00 Paper 98e: Programmable Metals: Metal-Graphene Catalytic Condenser — ***Tzia Ming Onn***, *Omar Abdelrahman, Phillip Christopher, K. Andre Mkhoyan, Matthew Neurock, C. Daniel Frisbie, Paul Dauenhauer*

2:18 Paper 98f: Identification of Highly Selective Surface Pathways for Methane Dry Reforming Using Mechano-Chemical Synthesis of Pd-CeO_2 — ***Juan D. Jimenez***, *Luis E. Betancourt, Maila Danielis, Hong Zhang, Ping Liu, Alessandro Trovarelli, Jose A. Rodriguez, Sara Colussi, Sanjaya D. Senanayake*

2:36 Paper 98g: Ceria Enhancement of Sinter-Resistant Platinum-Based Catalysts for Emission Control Applications — ***Michael Stone***, *Aisulu Aitbekova, Miaofang Chi, Simon Bare, Matteo Cargnello*

(99) Environmental Catalysis II: Fundamental Catalysis

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-227B

Erdem Sasmaz, Chair
Matteo Cargnello, Co-Chair

Sponsored by: Catalysis

12:30 Paper 99a: Activation of Lattice and Adatom Oxygen By Highly Stable Ceria-Supported Cu Single Atoms — *Carlos G. Vargas,* ***Gregory Collinge***, *Dongmin Yun, Mal-Soon Lee, Valery Muravev, Ya-qiong Su, Xavier Isidro Pereira Hernández, Dong Jiang, Vassiliki-Alexandra Glezakou, Emiel Hensen, Roger Rousseau, Abhaya Datye, Yong Wang*

12:50 Paper 99b: Evaluation of Low-Temperature Methane Oxidation Reaction over Pd Single-Atom Catalysts — ***Musa Najimu***, ***Erdem Sasmaz***

1:10 Paper 99c: Microkinetic Analysis of Low Temperature Nitrous Oxide Formation on Pt: Understanding the Role of Catalyst Surface Structure and Coverage — ***Sugandha Verma***, *Carlos Weiler, Robert J. Davis, William Epling, Christopher Paolucci*

1:30 Paper 99d: Mechanistic Studies of NH3-Assisted Reduction of Mononuclear Cu(II) Cation Sites in Cu-CHA Zeolites — ***Siddarth Krishna***, *Laura Wilcox, Casey B. Jones, Rajamani Gounder*

1:50 Paper 99e: Reductant Induced Redox Behavior of Atomically-Dispersed Palladium in Pd-CHA — ***Surya Pratap Solanki***, *Mugdha Ambast, Christopher Paolucci, Michael Harold, Lars Grabow*

2:10 Paper 99f: Comparative Studies of the Catalytic Behaviors By Ferrite-Based Single-Atom Catalysts for CO Oxidation in Thermal and Magnetic Induction Heating Reactors — ***Alexander Adogwa***, *Ewa Chukwu, Owen Chamness, Bridget Bruce, Olin Mefford, Ming Yang*

2:30 Paper 99g: Synthesis of Cu-Impregnated MFI Zeolite As Hydrocarbon Adsorbents; The Effective Roles of Cation — ***Jaehee Shim**, Jinseong Kim, Jungkyu Choi*

(100) Fundamentals of Catalysis and Surface Science II: Zeolites and acid catalysis

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-128B

Omar Abdelrahman, Chair
Yang Xiao, Co-Chair

Sponsored by: Catalysis

12:30 Paper 100a: Irreversible Adsorbate Thermodynamics on Zeolite Surfaces — ***Ajibola Lawal**, Omar Abdelrahman*

12:48 Paper 100b: Origins of Changes in Methanol Dehydration Turnover Rates on Brønsted Acid Sites in Zeolites with Different Al Distributions — ***Alexander Hoffman**, Ryoh-Suke Sekiya, John Di Iorio, Claire Nimlos, Rajamani Gounder, David Hibbitts*

1:06 Paper 100c: Mechanistic Insights on the Dehydration of Polyols over Bronsted Acid Sites — ***Quy Nguyen**, Steven Crossley, Bin Wang*

1:24 Paper 100d: Polyol Hydrodeoxygenation over Molybdenum Carbide Catalysts: From Surface Science to Liquid-Phase Reactor Environments — *Salai C. Ammal, **Andreas Heyden***

1:42: Break

2:00 Paper 100f: The Role of Acids and Redox Sites during Oxidative Scission of Ketones over $VO_x/\gamma\text{-}Al_2O_3$ — ***Bowei Liu**, Ran Zhu, Siwen Wang, Jesse Bond*

2:18 Paper 100g: Selective Oxidation of Ethanol over Zeolite-Supported Gold Catalysts — ***Yiteng Zheng**, Bruce E. Koel, Simon G. Podkolzin, Yue Qi, Jun Zhi Tan*

2:36 Paper 100h: Spectrokinetic Studies of Intermediate Species during Ethanol Oxidation on Supported Gold Catalysts — ***Alejandra Torres-Velasco**, Bhagyesha Patil, **Juan Bravo-Suarez***

(101) Microporous and Mesoporous Materials III: Structure

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-128A

Praveen Bollini, Chair
Joshua Howe, Co-Chair
Peng Bai, Co-Chair

Sponsored by: Catalysis

12:30 Paper 101a: Effects of Lewis Acidity and Confinement on Aldol Reactions of Aldehydes in Zeotypes — ***Wenlin He**, David Potts, David Flaherty, Viktor Cybulskis*

12:48 Paper 101b: Acid Catalysis over Low-Silica Faujasite Zeolites — ***Xinyu Li**, He Han, Wenqian Xu, Son-Jong Hwang, Zhichen Shi, Peng Lu, Aditya Bhan, Michael Tsapatsis*

1:06 Paper 101c: Unraveling the Complex Relationship between Framework Topology and Acidity on the Light Olefins Selectivities in the Methanol-to-Olefins Reaction — ***Faisal Alshafei**, Youngkyu Park, Stacey Zones, Mark Davis*

1:24 Paper 101d: Investigating Cyclization and Dehydrogenation Routes Toward the Conversion of Aromatic Compounds during Methanol-to-Olefins in MFI Framework Zeolites — ***Hansel Montalvo-Castro**, Lauren Kilburn, Mykela DeLuca, David Hibbitts*

1:42 Paper 101e: Mapping Interactions between Cationic Structure-Directing Agents and Framework Anions in Zeolites Using Computational Tools — ***Alexander Hoffman**, Songhyun Lee, Elizabeth Bickel, Claire Nimlos, Rafael Gomez-Bombarelli, Rajamani Gounder, David Hibbitts*

2:00 Paper 101f: Upgrading Biomass Using Cooperative Interactions in Aminosilica Materials for Aldol Condensation: Discovering Different Types of Catalytic Sites in Aminosilica Materials — ***Jee-Yee Chen**, Nicholas Brunelli*

2:18 Paper 101g: Impact of Zeolite Framework and Solvent Molecules on Vapor-Phase Propylene Epoxidation with Gaseous H_2O_2 — ***Ohsung Kwon**, E. Zeynep Ayla, David Potts, David Flaherty*

2:36 Paper 101h: Studies on Ag-Modified ZSM-5 Zeolite for Alkanes Catalytic Cracking and Its Reaction Mechanism — ***Xinyang Zhang***

(102) Intellectual Property for Practicing Engineers: Patents and Trade Secrets

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-225B

Paul Townsend, Chair
Lauren Dowty, Co-Chair

Sponsored by: Chemical Engineering & the Law Forum

12:30 Paper 102a: Intellectual Property and the Circular Economy — ***Paul Townsend**, **Lauren Dowty**, Charles Collins-Chase*

1:00 Paper 102b: Protecting Ideas in Joint Research Projects — ***Robert Sovesky***

1:30: General Discussion on Intellectual Property

(103) Recent Advances in Molecular Simulation Methods

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-222B

Michael Howard, Chair
Gul H. Zerze, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

12:30 Paper 103a: Brownian Bridges for Stochastic Chemical Processes – Applications and Approximation Method — ***Vivek Narsimhan**, Shiyan Wang, Anirudh Venkatesh, Doraiswami Ramkrishna*

12:45 Paper 103b: Supervised Learning and the Finite-Temperature String Method for Computing Committor Functions and Reaction Rates — ***Muhammad Hasyim**, Clay Batton, Kranthi K. Mandadapu*

1:00: Break

1:15 Paper 103d: Systematic Control of Collective Variables Learned from Variational Autoencoders — ***Jacob I. Monroe**, Vincent K. Shen*

1:30 Paper 103e: Accelerated Free Energy Calculations By Joint Biasing in Configurational and Alchemical Space in Metadynamics — ***Wei-Tse Hsu**, Pascal Merz, Giovanni Bussi, Michael Shirts*

1:45 Paper 103f: Exploring Low-Energy Regions of Glassy Potential Energy Landscapes — ***Amruthesh Thirumalaiswamy**, Robert Riggleman, John C. Crocker*

2:00 Paper 103g: Ordinary Least Squares, Extraordinary Overconfidence: Towards Improved Statistical Estimators for Particle Diffusivity — ***Kevin S. Silmore**, Yuanhao Li, Gerald J. Wang*

2:15 Paper 103h: How to Quantify Spatial Variations in Diffusivity in Molecular Dynamics Simulations. — ***Tiago Domingues**, Ronald Coifman, Amir Haji-Akbari*

2:30 Paper 103i: Leveraging the Wolf Method for Electrostatics to Extend Time and Length Scales Accessible By Monte Carlo Simulations — ***Gregory Schwing**, Mohammad Soroush Barhaghi, Brad Crawford, Loren Schwiebert, Jeffrey Potoff*

2:45 Paper 103j: py-MCMD: Hybrid Monte Carlo – Molecular Dynamics Simulations — ***Brad Crawford**, Mohammad Soroush Barhaghi, Gregory Schwing, David Hardy, John Stone, Loren Schwiebert, Jeffrey Potoff, Emad Tajkhorshid*

(104) Advances in Mixed-Integer Optimization and Optimization with Logistics Applications

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, W-101C

Pedro Castro, Chair
Venkatachalam Avadiappan, Co-Chair

Sponsored by: Systems and Process Operations

12:30 Paper 104a: Hybrid Mixed-Integer Programming/Constraint Programming Solution Strategies for Single-Stage Scheduling Problems Using a Discrete-Time Grid — ***Nathan Adelgren**, Christos T. Maravelias*

12:48 Paper 104b: Extending Generalized Disjunctive Programming to Model Hierarchical Systems — ***Hector Perez**, Seolhee Cho, Ignacio Grossmann*

1:06 Paper 104c: Tightening Discretization-Based MILP Models for the Pooling Problem Using Upper Bounds on Bilinear Terms — ***Yifu Chen**, Christos Maravelias*

1:24 Paper 104d: A Hybrid Multicut Generalized Benders Decomposition Algorithm for the Integration of Process Operations and Dynamic Optimization — ***Ilias Mitrai**, Prodromos Daoutidis*

1:42 Paper 104e: *A Priori* Objective Dimensionality Reduction for Many-Objective Optimization — ***Justin Russell**, Andrew Allman*

2:00 Paper 104f: Piecewise Linear Decision Rules Via Adaptive Partition for Two Stage Stochastic Mixed Integer Linear Programs — ***Can Li**, Kibaek Kim*

2:18 Paper 104g: Reformulation and Decomposition of Integer Programs Using Propositional Logic — ***Chinmay Aras**, M M Faruque Hasan*

2:36 Paper 104h: Surrogate-Based Optimization for Box-Constrained Black-Box Systems Via k-Means Clustering — ***Maaz Ahmad**, Iftekhar Karimi*

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(105) CAST Director's Student Presentation Award Finalists (Invited Talks)

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, W-101A

Rahul Bindlish, Chair

Sponsored by: Computing Systems and Technology Division

12:30 Paper 105a: Development of an Integrated Multiscale Modeling, Experimental, and Control Framework for Commercialization of Quantum Dot Manufacturing and Their Applications — ***Niranjan Sitapure**, Joseph Kwon*

12:45 Paper 105b: Machine Learning-Enabled Optimization of Classical Molecular Models — ***Bridgette Befort**, Ryan S. DeFever, Edward Maginn, Alexander Dowling*

1:00 Paper 105c: Discovering First-Principles-Based Models Using Machine Learning for Physicochemical Systems — ***Arijit Chakraborty**, Venkat Venkatasubramanian*

1:15 Paper 105d: Deep Kernel Distributionally Robust Joint Chance-Constrained Process Optimization — ***Shu-Bo Yang**, Zukui Li*

1:30 Paper 105e: Developing Roadmaps to Guide Industry Toward a Future with Net-Zero Emissions and a Circular Economy — ***Vyom Thakker**, Bhavik Bakshi*

1:45 Paper 105f: Cyberattack Detection and Handling Strategies with Online Data-Gathering Capabilities Using Lyapunov-Based Economic Model Predictive Control — ***Henrique Oyama**, Keshav Kasturi Rangan, Helen Durand*

2:00 Paper 105g: Dynamic Scheduling of Batch Operations and Customer Order Transactions in a Chemical Supply Chain — ***Hector Perez**, John Wassick, Ignacio Grossmann*

2:15 Paper 105h: Optimizing the Food-Energy-Water Nexus – from Surrogate Modeling to Informed Decision-Making — ***Marcello Di Martino**, Patrick Linke, Efstratios N. Pistikopoulos*

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(106) Data-Driven Dynamic Modeling, Estimation and Control II

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, W-101B

Zhenyu Wang, Chair
Heleno Bispo, Co-Chair

Sponsored by: Systems and Process Control

12:30 Paper 106a: Building a Large-Scale Kinetic Model for *Saccharomyces Cerevisiae*: Challenges and Insights — ***Mengqi Hu**, Hoang Dinh, Yihui Shen, Charles Foster, Patrick Suthers, Joshua D. Rabinowitz, Costas D. Maranas*

12:49 Paper 106b: Hybrid Modeling of Bioprocesses Based on a Kinetic Canonical Formalism — ***Tim Forster**, Daniel Vázquez, Mariano Nicolas Cruz Bournazou, Alessandro Butté, Gonzalo Guillén-Gosálbez*

1:08 Paper 106c: Inverse Backward Analysis of Neural Approximants of Ordinary Differential Equations — *Thomas Bertalan, Aiqing Zhu, Beibei Zhu, Yifa Tang,* ***Ioannis G. Kevrekidis***

1:27 Paper 106d: Experimental Demonstration of Closed-Loop Optimization of a Single Column Pressure Swing Adsorption (PSA)-Based Oxygen Concentrator Using Machine Learning — ***Zeping Chen**, Andrew Branen, Mayuresh Kothare, Gautam Kumar*

1:46 Paper 106e: Nonlinear Reactor Design Optimization with Embedded Microkinetic Model Information for Sustainable Shale Gas Processing — ***Kanishka Ghosh**, Santiago Salas, Jennifer B. Dunn, Alexander Dowling*

2:05 Paper 106f: Deep Learning Aided Koopman Predictive Control for Post-Combustion CO_2 Capture Process — *Xuewen Zhang, Benjamin Decardi-Nelson,* ***Xunyuan Yin***

2:24 Paper 106g: Development of Algorithms for Augmenting and Replacing Conventional Process Control Using Reinforcement Learning — ***Daniel Beahr**, Matthew Alastanos, Elijah Hedrick, Debangsu Bhattacharyya*

2:43 Paper 106h: Data-Driven Predictive Control of Two-Timescale Dynamics: Application to a Battery System — ***Bhavana Bhadriraju**, Joseph Kwon, Faisal Khan*

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(107) Assessment and Evaluation of Student Learning and Performance

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, W-105B

Lucas Landherr, Chair
Jennifer Weiser, Co-Chair
Adam K. Ekenseair, Co-Chair

Sponsored by: Education

12:30: Welcoming Remarks

12:32 Paper 107a: The World Is Changing and We Must Change with It - Lessons Learned in Alternative Grading Approaches in Core Chemical Engineering Courses — ***Daniel Burkey**, **Jennifer Pascal**, **Matthew Stuber**, **Kristina Wagstrom***

12:50 Paper 107b: Implementation of Achievement-Based Grading in Chemical Engineering Core Classes — ***Adam K. Ekenseair***

1:08 Paper 107c: Perspectives on Alternative Assessment in Core Chemical Engineering Courses — ***Joshua Enszer***

1:26 Paper 107d: Ungrading in Process Control: Attempting to Eliminate Exams, Deadlines, and Anxiety By Refocusing on Learning Instead of Grades — ***Lucas Landherr***

1:44 Paper 107e: Efficacy and Perceptions of a Specifications Grading Scheme for Chemical Engineering Seniors — ***David Wagner***

2:02 Paper 107f: Assessing Authentic Problem-Solving in Heat Transfer — ***Jiamin Zhang**, Soheil Fatehiboroujeni, Matthew Ford, Eric Burkholder*

2:20 Paper 107g: Assessment of an Inquiry-Based Learning Bioadhesive Module to Teach Principles of Tissue Repair — *Chris Panebianco, Poorna Dutta, Jillian Frost, Angela Huang,* ***Olivia Kim**, James Iatridis, Andrea Vernengo, Jennifer Weiser*

2:38 Paper 107h: Comparing Formative and Summative Auto-Graded Problems for a Material and Energy Balances Course — *Samantha Yanosko,* ***Matthew Liberatore***

(108) Computing and Data Science in ChE Education

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, W-105C

Amanda Simson, Chair
Manuela Ayee-Leong, Co-Chair

Sponsored by: Undergraduate Education

12:30: Welcoming Remarks

12:32 Paper 108a: Computing and Data Analytics through Problem Based Learning — ***Weiguo Xie***, *Richard Davis*

12:50 Paper 108b: Teaching Process Simulation Concepts in Aspen Plus Using the Ammonia Synthesis Loop — ***Jason White***

1:08 Paper 108c: Deliberate Practice of Spreadsheet Skills Using Randomized, Auto-Graded Problems — *Luke Gorbett, Kayla Chapman,* ***Matthew Liberatore***

1:26 Paper 108d: Python for Chemical Engineering Calculations: An Elective Course for Undergraduate Students — ***Gennady Gor***

1:44 Paper 108e: Experience with Symbolic Algebra and Smart Computing in Chemical Engineering Curriculum — ***Satish Parulekar***

2:02 Paper 108f: Open Source Python-Based Application As an Interactive Spectroscopic Teaching Aid — ***Jakub Konkol***, *George Tsilomelekis*

2:20 Paper 108g: Hello World of (Bio)Chemical Engineers: A Structured and Tailored Python Course — ***Fiammetta Caccavale***, *Carina L. Gargalo, Krist V. Gernaey, Ulrich Krühne*

(109) NSF Workshop I: Highlights from CBET

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, W-105A

Ram Gupta, Chair
Carole Read, Co-Chair

Sponsored by: Career Guidance Committee Liaison

12:30 Paper 109a: Division Director Update on the Chemical, Bioengineering, Environmental, and Transport Systems Division of NSF: Programs and Opportunities — ***Jeanne VanBriesen***

12:55 Paper 109b: Briefing of the Chemical Process Systems Cluster of the CBET Division of the National Science Foundation — ***Ray Adomaitis***

1:15 Paper 109c: Update on Programs in the Transport Phenomena Cluster of the CBET Division of NSF — ***Shahab Shojaei-Zadeh***

1:35 Paper 109d: Update on Programs of the Engineering Biology and Health Cluster of the NSF CBET Division — ***Steven Peretti***

1:55 Paper 109e: Update on Programs of the Environmental Engineering and Sustainability Cluster of the CBET Division of NSF — ***Mamadou Diallo***

2:15 Paper 109f: Interactive Question and Answer Session with NSF Program Directors — ***Carole Read***, *Jeanne VanBriesen, Ray Adomaitis, Shahab Shojaei-Zadeh, Steven Peretti, Mamadou Diallo*

(111) Active Colloidal Systems

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-232A

Ubaldo M. Córdova-Figueroa, Chair
Ilona Kretzschmar, Co-Chair

Sponsored by: Interfacial Phenomena

12:30 Paper 111a: Specific and Non-Specific Molecular Control of Catalytic Active Janus Particles — *Marola Issa, Diego Calderon, Olivia Kamlet, Julie N. Renner,* ***Christopher L. Wirth***

12:45 Paper 111b: Active Janus Particle Behavior at Oil/Water Boundaries — ***Baseemah Rucker***, *Ilona Kretzschmar, Alexander Couzis*

1:00: Break

1:15 Paper 111d: Curvature-Controlled Geometrical Lensing Behavior in Self-Propelled Colloidal Particle Systems — ***Philipp Schönhöfer***, *Sharon Glotzer*

1:30 Paper 111e: Active Surface Agents: Active Colloids at Fluid-Fluid Interfaces — *Jiayi Deng, Mehdi Molaei, Nicholas Chisholm,* ***Dr. Kathleen J. Stebe***

1:45 Paper 111f: Surface Topography Influences Driven Filament Alignment and Controls Swarm Formation — ***Kevin Modica***, *Joseph Barakat, Sho Takatori*

2:00 Paper 111g: Modulating the Drift of Rotary Active Particles and Microswimmers — ***Amir Nourhani***, *Mohammad Nabil, Andrew Frankowski, Ashton Orosa, Andrew Fuller*

2:15 Paper 111h: Emergent Microrobotic Oscillators Via Asymmetry-Induced Order — ***Jing Fan Yang***, *Thomas Berrueta, Allan Brooks, Albert Tianxiang Liu, Ge Zhang, Sungyun Yang, Volodymyr Koman, Todd Murphey, Michael Strano*

2:30 Paper 111i: Morphogenesis of Growing Bacterial Colonies in Polymeric Environments — *Sebastian Gonzalez La Corte, Tapomoy Bhattacharjee, Brianna Royer, Ned Wingreen,* ***Sujit Datta***

(112) Area Plenary: Symposium in Memory of James W. Swan (Invited Talks)

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-229AB

Matthew Helgeson, Chair

Sponsored by: Fluid Mechanics

12:30 Paper 112a: Introductory Remarks - Jim Swan: Scholar, Colleague, Friend — ***Matthew Helgeson***

12:40 Paper 112b: Swimming in Potential Flow — ***John Brady***, *Alec Glisman*

1:00 Paper 112c: A Journey through Colloids and Friendship — ***Roseanna Zia***

1:20 Paper 112d: Dissipative Self-Assembly of Colloidal Dispersions — ***Eric Furst***

1:40 Paper 112e: Hydrodynamic Memory and Quincke Rotation — ***Aditya Khair***

2:00 Paper 112f: Controlling the Thermal Gelation of Nanoemulsions and Applications Thereof — ***Patrick Doyle***

2:20 Paper 112g: Self-Assembly and Optical Properties of Colloidal Dispersions in Electromagnetic Fields — ***Zachary Sherman***

2:40 Paper 112h: Jim Swan and Rheometry: Medium Amplitude Parallel Superposition (MAPS) Rheology — ***Gareth H. McKinley***

(113) Biomolecules at Interfaces I

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-232B

Roberto Andresen Eguiluz, Chair
Julie N. Renner, Co-Chair
Bernardo Yanez Soto, Co-Chair

Sponsored by: Interfacial Phenomena

12:30 Paper 113a: Mapping the Morphology of DNA Adsorbed on Carbon Nanotubes Using X-Ray Scattering Interferometry — ***Rebecca L. Pinals***, *Daniel J. Rosenberg, Joshua D. Hubbard, Natalie S. Goh, Francis J. Cunningham, Emily Hayman, Gregory Hura, Markita Landry*

12:45 Paper 113b: Zwitterionic Hydrogel Coatings Photografted to Biomaterial Surfaces Decrease Fibrotic Response and Increase Lubricity — ***Adreann Peel***, *Ryan Horne, Douglas Bennion, Megan Jensen, Marlan Hansen, Allan Guymon*

1:00 Paper 113c: Understanding the Role of Multivalent Counterions in the Interfacial Self-Assembly of Tripeptides — ***Gershon Starr***

1:15 Paper 113d: The Investigation of the Transition Temperature of Charged and Uncharged Elastin-like Polypeptides in Water and Salt Solutions By QCM-D — ***Sogol Asaei***, *Nuttanit Pramounmat, Julie N. Renner*

1:30: Break

1:45 Paper 113f: The Antagonistic Effect of Membrane Oxysterols on Bacterial Pore Forming Toxins — ***Samlesh Choudhury**, Aditya Upasani, Diksha Parwana, Rahul Roy, K. G. Ayappa*

2:00 Paper 113g: Rare Earth Element Recovery Is Only a 'Click' Away: Recovering Lanthanides with Peptide-Functionalized Polyvinylidene (PVDF) Membranes — ***Jacob Hostert**, Maura Sepesy, Christine Duval, Julie N. Renner*

2:15 Paper 113h: 3D Molecular Structures of Lanthanide Binding Peptides for Air-Water Interfacial Separation of Rare Earth Elements — ***Surabh KT**, Luis Ortuno, Denize Favaro, Raymond S. Tu, Charles Maldarelli, Robert Messinger*

2:30 Paper 113i: Continuous Nano-Thin Coating Formation By Silk Fibroin Self-Assembly — ***Caleb Wigham**, Tanner D. Fink, Padraic O'Reilly, Sung Park, Runye Zha*

(114) Emerging Topics in Electrochemical Engineering: Electrochemical Separations (Invited Talks)

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-232C

William Tarpeh, Chair
Christopher Arges, Co-Chair

Sponsored by: Electrochemical Fundamentals

12:30 Paper 114a: Redox-Tunable Lewis Bases for Electrochemical Carbon Dioxide Separation — ***Yayuan Liu***

1:05 Paper 114b: Modeling and Testing of Functionalized Interfaces for Electrochemical Separations — *Manh-Thuong Nguyen, Difan Zhang, Shuai Tan, Xuebin Wang, Venky Prabhakaran, Grant Johnson, Roger Rousseau,* ***Vassiliki-Alexandra Glezakou***

1:40 Paper 114c: Using Redox Couples to Enable Energy-Efficient Water Desalination and Nutrient Recovery — ***Taeyoung Kim**, Gowri Mohandass, Weikun Chen, Sitaraman Krishnan, Shane Rogers, Stefan Grimberg*

2:15 Paper 114d: Placeholder - Yushan Yan — ***Yushan Yan***

(115) New Frontiers of Molecular Thermodynamics (Invited Talks)

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-223

Shikha Nangia, Chair
Sapna Sarupria, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

12:30: Welcoming Remarks

12:32 Paper 115a: Guiding the Design of Ionic Liquids with Machine Learning — ***Jindal Shah***

1:05 Paper 115b: Protein Vesicles: Tuning Self-Assembly By Sequence Modifications — ***Julie Champion***

1:38: Break

1:48 Paper 115c: Predictive Modeling of Nanoporous Materials: Large-Scale Simulations, High-Throughput Screening and Machine Learning — ***J. Ilja Siepmann***

2:21 Paper 115d: To be Announced — ***Lola Eniola-Adefeso***

(116) Environmental Division Awards and Honors (Invited Talks)

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-224AB

Alexander Orlov, Chair
Kristina Wagstrom, Co-Chair

Sponsored by: Environmental Division

12:30 Paper 116a: Lawrence K. Cecil Award Winner Presentation: "Life-Cycle-Based Multiscale Sustainability: Challenges and Opportunities in the Era of Industry 4.0" — ***Yinlun Huang***

1:15 Paper 116b: Early Career Award Winner Presentation: "Enabling Solvent Recovery and Reuse via Systems Engineering and Synergistic Industry-Academia Collaborations" — ***Kirti Yenkie***

1:45 Paper 116c: Graduate Student Paper Award, 1st Place: "Enhancing CO Oxidation Activity via Tuning a Charge Transfer Between Gold Nanoparticles and Supports" — ***Haotian Yang***

2:00 Paper 116d: Grad Student Paper Award, 2nd Place: "A New Avenue for Separating Contaminants from Water using Nanofiltration and Adsorptive Materials" — ***Francisco Leniz-Pizarro***

2:15 Paper 116e: Grad Student Paper Award, 3rd Place: "Effect of Combustion Particle Morphology on Biological Responses in a Co-culture of Human Lung Epithelial and Macrophage-like Cells" — ***Kamaljeet Kuar***

(117) Biocatalysis and Enzyme Engineering

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-125A

Carl Denard, Chair
Nikhil Nair, Co-Chair

Sponsored by: Bioengineering

12:30 Paper 117a: Elucidating the Complex Interactions between Stability, Oligomericity, and Activity of α-Amino Ester Hydrolase — ***Colton Lagerman**, Martha Grover, Ronald Rousseau, Andreas Bommarius*

12:48 Paper 117b: Orthogonal Glycolytic Pathway Enables Directed Evolution of Noncanonical Cofactor Oxidase — *Edward King, Sarah Maxel,* ***Yulai Zhang**, Karissa Kenney, Gregory A. Weiss, Ray Luo, Han Li*

1:06 Paper 117c: Rank-Ordering of Known Enzymes As Starting Points for Re-Engineering Novel Substrate Activity Using a Convolutional Neural Network — ***Vikas Upadhyay**, Veda Sheersh Boorla, Costas D. Maranas*

1:24 Paper 117d: A High-Throughput Activity Screen for Reprogramming Proteases (HARP) — ***Samantha Martinusen**, Ethan Slaton, Cassidy Simas, Benjamin Stone, Carl Denard*

1:42 Paper 117e: Effects of Sequence Features on Machine-Learned Enzyme Classification Fidelity and Implications on *De Novo* enzyme Design — ***Md Sakib Ferdous**, Nigel Reuel*

2:00 Paper 117f: Engineered Cynr Regulon for Enzymatic Biocatalysis Enables Milk Oligosaccharides Biosynthesis Using Azido Sugars — *Chandra Kanth Bandi, Mohit Kumar,* ***Shishir Chundawat***

2:18 Paper 117g: Data Driven Biomolecular Engineering Using High Throughput Measurements of Protein Function — ***Timothy A. Whitehead***

(118) Biomolecular Engineering III

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-126A

Xue Gao, Chair
Ashish Kulkarni, Co-Chair
Whitney Stoppel, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

12:30 Paper 118a: All-Atom Molecular Dynamics Simulations of Poly-Ethylene-Glycol (PEG) and Limp-2 Reveal That Peg Penetrates Deep into the Proposed CD36 Cholesterol-Transport Tunn — ***Paul Dalhaimer**, Kate Blankenship*

12:48 Paper 118b: Molecular Simulations of Zwitterlation-Induced Conformation and Dynamics Variation of Glucagon-like Peptide-1 and Insulin — *Qi Qiao, Lirong Cai,* ***Qing Shao***

1:06 Paper 118c: Comparison of Three High-Level Microarray Statistical Analysis Methods for Disease Mechanism Identification — ***Dayna Schultz**, Ilias Frydas, Spyros Karakitsios, Dimosthenis Sarigiannis*

1:24 Paper 118d: Extending the Bioavailability of Hydrophilic Antioxidants for Metal Ion Detoxification Via Crystallization with Polysaccharide Dopamine — ***Ryan Miller**, Youngsam Kim, Chang Gyun Park, Young Jun Kim, Hyunjoon Kong*

1:42 Paper 118e: Lentiviral-Based Fluorescent Reporters for Assessing Human Lung Fibroblast Activation in Response to Microenvironmental Stimuli in Multidimensional Culture Systems — ***Samantha Cassel**, April Kloxin*

2:00 Paper 118f: Invited Talk: Placeholder for the Invited Talk in Biomolecular Engineering III Session — ***Whitney Stoppel***, *John Blazeck, Xue Sherry Gao*

(119) Cell and Tissue Engineering: Engineering 3D Tissues to Model Disease and Development

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-126B

Panagiotis Mistriotis, Chair
Laurel Hind, Co-Chair
Whitney Stoppel, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

12:30 Paper 119a: Developing an Ex Vivo Mesolimbic Pathway Model for Exploring Phenotypes Linked with Addiction — ***Thomas Rudibaugh***, *Albert J. Keung*

12:48 Paper 119b: Investigating Changes in Extracellular Matrix Architecture in a 3D Glioblastoma Model — ***Rosalyn Hatlen***, *Padmavathy Rajagopalan*

1:06 Paper 119c: Chemo-Therapeutic Screening on NOVEL Scaffold Assisted Dynamic *in Vitro* multicellular Models of Pancreatic Cancer — *Priyanka Gupta,* ***Melina Kitsiou***, *Pedro Perez-Mancera, Hemant Kocher, Andrew Nisbet, Giuseppe Schettino, Eirini Velliou*

1:24 Paper 119d: Secretome of Engineered Neuron-Innervated Muscle — ***Kai-Yu Huang***, *Gelson Pagan-Diaz, Young-Hak Cho, Sung Gap Im, Rashid Bashir, Hyunjoon Kong*

1:42 Paper 119e: Engineering an iPSC-Based 3D Liver Organoid for Hepatotoxicity Studies — ***Neeti Gandhi***, *Padmavathy Rajagopalan*

2:00 Paper 119f: Combined Cellular and Tissue Engineering Approaches for Functional Vascularization of Biomaterials — ***Mai T. Ngo***, *Ahmad S. Khalil, Christopher S. Chen*

2:18 Paper 119g: Invited Talk: Placeholder for the Cell and Tissue Engineering: Engineering 3D Tissues to Model Disease and Development — ***Whitney Stoppel***, *Panagiotis Mistriotis, Laurel Hind*

(120) Computational and systems biology tools for metabolic engineering and cell characterization

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-125B

Ross Thyer, Chair
Arul Mozhy Varman, Co-Chair
Cong Trinh, Co-Chair

Sponsored by: Bioengineering

12:30 Paper 120a: Are Genome Scale Metabolic Models (GeMs) Fit for Purpose? A Comprehensive Analysis into the Reliability of Chinese Hamster Ovary (CHO) Cell GeMs. — ***Benjamin Strain***, *James Morrissey, Cleo Kontoravdi*

12:48 Paper 120b: Quantification of Metabolic Differences in Platelets Exposed to Estrogen Using Flux Balance Analysis — ***Samantha Siska***, *Cara Sake, Alexander Metcalf, Nanette Boyle, Keith B. Neeves*

1:06 Paper 120c: Metabolic Modeling of Eicosapentaenoic Acid (EPA) and Arachidonic Acid (AA) Fatty Acids Using a Cybernetic Framework — ***Sana Khanum***, *Shakti Gupta, Rubesh Raja, Lina Aboulmouna, Naseeha Mohammed, Mano Maurya, Shankar Subramaniam, Doraiswami Ramkrishna*

1:24 Paper 120d: Design of Diverse, Functional Mitochondrial Targeting Sequences across Eukaryotic Organisms Using Variational Autoencoders — ***Aashutosh Boob***, *Nilmani Singh, Xueyi Xue, Airah Zaidi, Li-Qing Chen, Huimin Zhao*

1:42 Paper 120e: Next-Flux (Neural-net EXtracellular Trained Flux) — ***James Morrissey***, *Benjamin Strain, Gianmarco Barberi, Pierantonio Facco, Cleo Kontoravdi*

2:00 Paper 120f: Dgpredictor: Automated Fragmentation Method for Gibbs Energy Change Prediction of Metabolic Reaction and *De Novo* Pathway Design — ***Vikas Upadhyay***, *Costas D. Maranas*

2:18 Paper 120g: Multidimensional Resource Allocation Predicts Contrarian Reverse Diauxie Phenotype in *Pseudomonas Aeruginosa* — *S. Lee McGill, Yeni Yung, Kristopher A. Hunt, Luke Hanley,* ***Ross P. Carlson***

(121) Lignin for Sustainable Industrial Uses

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-228A

Manjusri Misra, Chair
Amar K. Mohanty, Co-Chair

Sponsored by: Forest and Plant Bioproducts Division

12:30 Paper 121a: Synthesis of Paracetamol and 4-Aminophenol from Lignin-Derived Hydroquinone — ***Jimin Park***, *Marta Hatzell, Carsten Sievers, Andreas Bommarius*

1:00 Paper 121b: Properties of Activated Carbon from Two Lignin Waste Streams in Lignocellulosic Biorefineries — ***Chengjun Wu***, *Graham W. Tindall, Carter Fitzgerald, Mark C. Thies, Mark E. Roberts*

1:30 Paper 121c: Biobased Composites for Improved Mechanical Performance and Recyclability — ***Xianglan Bai***, *Yixin Luo, Moham Razzaq, Baker Kuehl, Eric Cochran*

2:00 Paper 121d: Sustainable Green Composite Materials from Advanced Biocarbons: A Path Forward to Circular Bioeconomy — ***Manjusri Misra***

(122) Advances in Petroleum Production and Refining

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, W-103A

M R Riazi, Chair
Vladimir Mahalec, Co-Chair

Sponsored by: Fuels and Petrochemicals Division

12:30 Paper 122a: Welcoming — ***M R Riazi***, *Vladimir Mahalec*

12:33 Paper 122b: Advanced Parameter Estimation for Motor Gasoline Blending — *Jeffrey D. Kelly,* ***Brenno Menezes***

12:48 Paper 122c: Experimental and Numerical Studies on the Phenomena of Interfacial Mixing in Pipelines Processing Lube-Oil — ***Swapana Jerpoth***, *Robert Hesketh, C. Stewart Slater, Mariano J. Savelski, Kirti Yenkie*

1:03 Paper 122d: Preventing H_2S Poisoning of Pd Membranes for H_2 Purification Using Applied Electric Fields — ***Daniel J. Rivera***, *Christopher Muhich*

1:18 Paper 122e: Understanding Catalyst Failure Mechanisms in Plant Operation — ***Jin Yang***, *Vera Santos, Ewa Tocha, David G. Barton, Eric Stangland, Daniel Grohol, van Bloois Stefan, Joost Depicker, Ailene G. Phillips, Michael B Dr Clark, Leadley Stuart*

1:33 Paper 122f: Strategies for Systematically Optimizing the Operational Management of Lube-Oil Manufacturing and Packaging Facilities — ***Swapana Jerpoth***, *Robert Hesketh, C. Stewart Slater, Mariano J. Savelski, Kirti Yenkie*

1:48 Paper 122g: Demulsification of Tight Crude Oil-Water Emulsions Under Microwave Radiation in Presence of Nanohybrid Hydrophilic Structures — ***Prasad Pawar***, *Pankti Joshi, Clayton Jeffryes*

2:03 Paper 122h: Screening and Investigation on Inhibition of Sediment Formation in a Kuwait Light Crude Oil By Commercial Additives with Some Guidelines for Field Applications — *Ali Qubian, A.S. Abbas, N. Al-Khedhair, Jose Peres, O. Alomair, D. Stratiev, I. Shishkova,* ***M R Riazi***

2:15 Paper 122i: Crude Assays - the Distillation — ***Andrew Sloley***

2:27 Paper 122j: Mechanistic Investigation of Asphaltene-Induced Fouling of Heat Exchangers — ***Yousef Al-Shamlan***

2:38 Paper 122k: Dual Functional Catalysts for Cracking of Light Cycle Oil into Monoaromatics Using a Hydrogen Donor — ***Akshata Ramteke***, *Dwijraj Mhatre, Divesh Bhatia, Kamal Pant*

2:49 Paper 122l: Cracking of Light Cycle Oil in Presence of Hydrogen Donor into BTX Fraction — ***Akshata Ramteke**, Divesh Bhatia, Kamal Pant*

(123) Developments in Electrochemical Reactors, Fuel Cells, and Electrolyzers II

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, W-102C

Jamelyn Holladay, Chair
Helen Lou, Co-Chair

Sponsored by: Fuels and Petrochemicals Division

12:30: Welcoming Remarks

12:35 Paper 123a: A Co-Axial Microtubular Electrochemical Flow Cell for High-Power Flow Batteries and Electrolyzers — ***Nian Liu***

12:55 Paper 123b: High Performance Direct Methanol Fuel Cells Incorporating pH-Gradient-Enabled Microscale Bipolar Interfaces — ***Kritika Sharma**, Shrihari Sankarasubramanian, Zhongyang Wang, Vijay Ramani*

1:15 Paper 123c: Intensifying Thermocatalytic Methanol Synthesis Using Electrochemical H_2 Activation — ***Samantha Roenigk**, Evan Miu, Manjodh Kaur, James R. McKone*

1:35 Paper 123d: Separation of diluted ethanol produced by CO_2 electrolysis can be cost effective — ***Magda Barecka**, Joel W. Ager III, Alexei A. Lapkin*

1:55 Paper 123e: Model-Based Development of a Novel Apparatus for Electrochemically Induced Crystallization of (di-)Carboxylic Acids — *Jonas Goertz, **Kristina Mielke**, Marcel Gausmann, Andreas Jupke*

2:15 Paper 123f: Investigation of Current Production and Metal Removal from Synthetic Desalter Effluent Using a Dual Chamber Microbial Fuel Cell (MFC) with *Shewanella Oneidensis* MR-1 — ***Carlos Munoz**, Amarjeet Bassi*

2:35: Concluding Remarks

(124) Materials for Thermochemical and Electrochemical Energy Storage

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-228B

Anirudh Balram, Chair
Jian Liu, Co-Chair
Yunfa Chen, Co-Chair

Sponsored by: Green Process and Product Engineering

12:30 Paper 124a: Ammonium Formate As a Safe, Energy-Dense Electrochemical Fuel Ionic Liquid — ***Zachary Schiffer**, Sayandeep Biswas, Karthish Manthiram*

1:00 Paper 124b: Fossil Fuel Assets and Wastewater Resources Integrated SOLID OXIDE Electrolytic Cell for a NOVEL Hydrogen Production — ***Lateef Jolaoso**, Javad Asadi, Pejman Kazempoor*

1:30 Paper 124c: Enhanced Phase Change Materials for Ocean Thermal Energy Conversion — ***Jian Liu**, Brianna Friedman, Hyunjun Jung, Aljon Salalila, Habilou Ouro-Koura, Daniel Z. Deng*

2:00 Paper 124d: Substituted Zeolites As Promising O_2 Sorption Pump Materials: A Density Functional Theory Study — ***Steven Wilson**, Ellen B. Stechel, Ivan Ermanoski, Christopher L. Muhich*

2:30 Paper 532by: Investigation of the Thermochemical Reaction Pathways of Solid-State Ammonia Borane with Chemical Oxidizers — ***Prithwish Biswas**, Hyuna Kwon, Bryan M. Wong, Michael Zachariah*

(125) Technologies for Understanding Microbial Interactions

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-222A

Tagbo Niepa, PhD, Co-Chair
Elizabeth Stewart, Co-Chair
Sricharani Balmuri, Co-Chair
Warren Ruder, Co-Chair

Sponsored by: Miscellaneous

12:30 Paper 125a: Efficient Bacterial mRNA Sequencing in Diverse Species and Co-Cultures — ***Kellie Heom**, Chatarin Wangsanuwat, Lazarina Butkovich, Michelle O'Malley, Siddharth Dey*

12:55 Paper 125b: Development of a Gut-Inducible Expression Toolkit for Engineering in Probiotic Yeast *Saccharomyces Boulardii* — ***Deniz Durmusoglu**, Nathan Crook*

1:20 Paper 125c: Engineered Habitats for Understanding Fungal Growth in Soil — ***Yi-Syuan Guo**, Gregory Bonito, Scott T. Retterer*

1:45 Paper 125d: Mini-Bioreactors for the Study of Pneumococcal Cell-Cell Communication — ***Corine Jackman Burden**, Lydia Eutsey, Frederick Lanni, Shelley L. Anna, Luisa Hiller*

2:10 Paper 125e: Heterogeneous Bacterial Energies As a Bet-Hedging Strategy Against Antibiotics — ***Pushkar Lele***

(126) Undergraduate Research Presentations - Energy, Materials, and Petrochemicals

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-231C

Cory Thomas, Chair

Sponsored by: Young Professionals Committee (YPC)

(127) Leading and Managing Industry-Academia Collaborations and Partnerships

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, W-102B

Aditi Khadilkar, Chair
Harold Conner Jr., Co-Chair

Sponsored by: Management Division

12:30 Paper 127a: Establish Psychological Safety to Enhance Team Creativity, Inclusivity and Retention — ***Dennis Hess***

(128) Area Plenary: Leaders in Biomaterials (Invited Talks)

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-121B

Steven Caliari, Chair
Shreyas Rao, Co-Chair
Michael Gower, Co-Chair
Catherine Fromen, Co-Chair

Sponsored by: Biomaterials

12:30 Paper 128a: A Molecular Approach to Additive Manufacturing Medical Devices for Use in the Clinic — ***Matthew Becker***

1:20 Paper 128b: Biomaterials for Photothermal Tissue Sealing and Repair — ***Kaushal Rege***

2:10 Paper 128c: Self-Assembly and Applications of DNA-Amphiphiles — ***Efrosini Kokkoli***

(129) Charged and Ion Containing Polymers II

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-122A

Allie Obermeyer, Chair
Hee Jeung Oh, Co-Chair
Chibueze Amanchukwu, Co-Chair
Christian Aponte-Rivera, Co-Chair

Sponsored by: Polymers

12:30 Paper 129a: Chemical Determinants of Complexation in Polyelectrolyte Complex Coacervates — *Jun Huang, **Jennifer Laaser***

1:00 Paper 129b: Development of Poly(ionic liquid) Ionogels for Electroactive Polymer Application. — ***Kayla Foley**, Keisha Walters*

1:15 Paper 129c: Bridging the Gap between Scattering Results from Simulations and Experiments for Polyampholytes — ***Rohan Adhikari Sridhar**, Winnie Shi, Walter Chapman, Dilip Asthagiri, Amanda Marciel*

1:30 Paper 129d: Manufacturing and Remanufacturing of Ion-Mediated Polymer Assemblies, Blends and Nanostructures — ***Shuyi Xie**, Rachel Segalman*

1:45 Paper 129e: A Study of the Thermodynamics of PEO/PMMA /Litfsi Blend Electrolytes — ***Neel Shah***, *Lilin He, Kevin W. Gao, Marwan Shalaby, Bruce A. Garetz, Nitash P. Balsara*

2:00 Paper 129f: Investigation on Tethered Anion Effects in Solid Polymer Electrolytes for Li-Ion Conduction — ***Anthony Engler***, *Habin PARK, Nian Liu, Paul Kohl*

2:15: Break

2:30 Paper 129h: Counter-Ion Condensation on Doped *Π*-Conjugated Polymer Chains — ***Jaeyub Chung***, *Mahesh Mahanthappa, C. Daniel Frisbie*

2:45 Paper 129i: Synthesis, Purification, and Solution Properties of Net Anionic Poly(β-amino ester)s — ***Mara Kuenen***, *Alexa Cuomo, Rachel Letteri*

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(130) Inorganic Materials for Electrochemical Energy Storage

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-122B

Nian Liu, Chair
Yuzhang Li, Co-Chair

Sponsored by: Inorganic Materials

12:30 Paper 130a: Interfacial Stability of Al^{3+} and Ga^{3+} Dopants at the Lithium Garnet (M^{3+}-$Li_{6.5}La_3Zr_2O_{12}$) | Lithium Metal Interface — ***Matthew Klenk***, *Michael Counihan, Zachary Hood, Justin Connell, Sanja Tepavcevic, Peter Zapol*

12:51 Paper 130b: Improvements in Performance and Cost Reduction of Large-Scale Rechargeable Zinc|Manganese Dioxide Batteries and a Future Roadmap Driven through Real World Applications — ***Gautam Yadav***, *Jinchao Huang, Meir Weiner, Shinju Yang, Kristen Vitale, Sanbir Rahman, Kevin Keane, Sanjoy Banerjee*

1:12 Paper 130c: Understanding the Onset of Surface Degradation in Layered Li-Battery Cathodes — ***Xinhao Li***, *Wing-Chi Ashley Lam, In Won Yeu, Abhiroop Mishra, Joaquín Rodríguez-López, Alexander Urban*

1:33 Paper 130d: Facile Synthesis of Cos Nanoparticles Anchored on the Surface of Functionalized Mwcnts As Cathode Materials for Advanced Li-S Batteries — ***Zhao Wang***, *Wenduo Zeng, K.Y. Simon Ng*

1:54 Paper 130e: Interphase on Lithium Metal Anode Via Liquid Electrolyte Additives — ***Juchen Guo***

2:15 Paper 130f: Recent Developments in Operando Ultrasonic Characterization to Investigate Lithium Metal Cell Dynamics — ***Wesley Chang***

2:36 Paper 130g: Tailoring Ion Solvation Environment in Porous Polymer Electrolytes — ***Kaitlyn Engler***, *Jeffrey A. Reimer, Jeffrey R. Long*

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(131) Polymer Simulations: Structure and Fundamental Insights

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-121C

Poornima Padmanabhan, Chair
Thomas Gartner III, Co-Chair
Wenlin Zhang, Co-Chair
Janani Sampath, Co-Chair
Dylan Anstine, Co-Chair

Sponsored by: Polymers

12:30 Paper 131a: Thermodynamic Insights into the Reentrant Phase Behavior of a Copolymer Model — ***Yiming Wang***, *Frank H. Stillinger, Pablo Debenedetti*

12:45 Paper 131b: Coarse-Grained Models for Block Bottlebrush Polymer Self-Assembly — *Tianyuan Pan, Sarit Dutta,* ***Charles Sing***

1:15 Paper 131c: Coarse-Grained Molecular Dynamic Simulation of PS-PMMA Block Copolymer Directed Self-Assembly on a Flexible Brush Substrate — ***Yufeng Qiu***, *Yong Joo*

1:30 Paper 131d: Elucidating the Role of Network Topology Dynamics on the Coil-Stretch Transition Hysteresis in Extensional Flow of Entangled Polymer Melts — ***Mahdi Boudaghi***, *Mohammad Hadi Nafar Sefiddashti, Brian J Edwards, Bamin Khomami*

1:45 Paper 131e: Computational Design of Feather-like 2-D Polymer Architectures — ***Esmat Mohammadi***, *Soumil Joshi, Sanket Deshmukh*

2:00 Paper 131f: Diffusive Charge Transport in High-Valency Redox-Active Polymer Solutions — ***Liliana Bello Fernandez***, *Charles Sing*

2:15 Paper 131g: A Tunable, Particle-Based Model for the Diverse Conformations Exhibited By Chiral Block Polymers — ***Natalie Buchanan***, *Joules Provenzano, Poornima Padmanabhan*

2:30 Paper 131h: Designed Molecular Dynamics Investigation of the Thermal Conductivity and Mass Loss of Polyetherimide/Graphene Nanocomposites Exposed to Space Environments — ***Mohammad Mansourian-Tabaei***, *Shan Jiang,* ***Sasan Nouranian***

2:45 Paper 131i: Effect of Electric Field on PEO/Water Mixture: Molecular Dynamics Simulation Approach — ***Junhe Chen***, *Matthew Warner, Paul Kohl, Seung Soon Jang*

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(132) Carbon Nanomaterials I: Dispersion, Surface Structure, and Biointeractions

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, W-104B

Geyou Ao, Co-Chair

Sponsored by: Carbon Nanomaterials

12:30 Paper 132a: Investigating Serrs of Electrogenic Bacteria Via Charge Transfer Enhancement By Graphene Nano-Dots (GNDs) — ***Sheldon Cotts***, *Bijentimala Keisham, Roshan Nemade, Angelo Giles, Vikas Berry*

12:55 Paper 132b: Adsorption of Methylene Blue from Aqueous Solution By Zirconia Nanoparticles on Multiwall Carbon Nanotubes — ***Julian Lopez***, *Javier Lara Romero, Alexis Pérez Gasquez y Marín, Andrés Alejandro Damian Reyna*

1:20 Paper 132c: Graphene and MOS2 GEL for Aligned 3D Printing for Electronic and Mechanical Study — ***Deisy Cristina Carvalho Fernandes***, *Vikas Berry, Philippe Poulin*

1:45 Paper 132d: Modifiable Hydrogel Platform for the Delineation of Analyte Interactions on Individual Single-Walled Carbon Nanotubes — ***Matthew Card***, *Daniel Roxbury*

2:10 Paper 132e: Graphene and Skin Cancer Interaction for Next Generation Diagnostic Devices — ***Kartikey Sharma***, *Vikas Berry, Roshan Nemade, Carolina Puyana, Lacey Zimmerman*

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(133) Nanomaterials for Energy Storage

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, W-104A

Ling Fei, Chair
Jay Park, Co-Chair
Seung Soon Jang, Co-Chair

Sponsored by: Nanomaterials for Energy Applications

12:30 Paper 133a: Nature-Derived Nanostructures for Sustainable Si Anode in High-Energy Li-Ion Batteries — ***Zheng Chen***

1:00 Paper 133b: Rational Design of Interphases to Enable High Energy Metal-Based Batteries — *Christopher Fetrow, Matthew Powell, Cameron Carugati,* ***Shuya Wei***

1:30 Paper 133c: Design and Synthesis of Hollow Nanostructures of Cocoon-like Carbon Encapsulating Porous and Magnetic Cores for Energy, Biomedical, and Environmental Application — ***Foroogh Rouhollahi***, *Amin Vossoughi, Howard Matthew, Da Deng*

1:45 Paper 133d: Sequestration of Sulfur in Facilely Manufactured Carbon Nanospheres through Sulfur Recrystallization As an Effective PATH for LONG CYCLE Life of Lithium Sulfur Batteries — ***Wissam Fawaz***, *Zhao Wang, K.Y. Simon Ng*

2:00 Paper 133e: Investigating the Diffusivity of Ionic Liquids in Solvent-in-Salt System Using Molecular Dynamics Simulation — *Ray Matsumoto, **Wei Zhao**, Xiaobo Lin, Ivan Popov, Alexei Sokolov, Peter Cummings*

2:15 Paper 133f: Enhancing the Oxidative Stability of Mxenes — *Xiaofei Zhao, Jodie Lutkenhaus, Miladin Radovic, **Micah Green***

2:30 Paper 133g: PEGDA-ZIF-8 Composite Electrolyte for All-Solid-State Lithium Metal Batteries — ***Zizhou He**, Joshua Goulas, Rayden Farmer, Belle Racca, Ling Fei*

(134) Advances in Computational Analyses of Mixing Processes

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-227C

John Thomas, Chair
David Lignell, Co-Chair

Sponsored by: North American Mixing Forum

12:30 Paper 134a: Mixing Time Determination in a Vessel with Rotating Basket (USP Dissolution Testing Apparatus 1) — ***Justin Pace**, Chadakarn Sirasitthichoke, Piero Armenante*

1:00 Paper 134b: Efficient Modeling of Polydisperse Solid-Liquid Suspensions in Stirred Tanks — ***Philipp Eibl**, Martin Fruhwirth, Christian Witz, Johannes G. Khinast*

1:30 Paper 134c: Optimization of a Full-Scale Disinfection Unit Using CFD at Pero WWTP in Milan — *Cesare Piacezzi, Giacomo Bellandi, Alejandro Claro Barreto, Roberta Muoio, Roberto Di Cosmo, Davide Scaglione, Usman Rehman, **Ingmar Nopens***

2:00 Paper 134d: Lattice-Boltzmann Computational Fluid Dynamics (CFD) Simulation of Jet Mixing in Tanks — *John Thomas, **Michael Poirier***

2:30 Paper 134e: Accelerating Biopharmaceutical Mixing Process Development with Hybrid Modeling and Computational Fluid Dynamics — ***Ross Kenyon***

(135) Fluidization: Experimental Investigation and Modeling of Fluidization Processes

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, W-106C

Sarah Mena, Chair
Runxia Cai, Co-Chair

Sponsored by: Fluidization and Fluid-Particle Systems

12:30 Paper 135a: A Structured Bubbling Phenomenon in Vertically Vibrated Binary Gas–Fluidized Beds — ***Jagan Mohan Sanghishetty**, Christopher Spitler, Qiang Guo, D. R. Nagaraj, Raymond Farinato, Chris Boyce*

12:50 Paper 135b: Novel Positron Imaging and Numerical Modelling of Bubbling Fluidised Beds: Toward an Improved Understanding of Pyrolysis-Based Waste Plastic Recycling — ***Dominik Werner**, Kit Windows-Yule*

1:10 Paper 135c: Fluidized Bed Drying of Supported Catalysts: Effect of Process Parameters — ***Carlin Leung**, Justin Adler, Tim A. G. Langrish, Benjamin Glasser*

1:30 Paper 135d: Stirrer Design for Improving Fluidization of Cohesive Powder — ***Kaiqiao Wu**, Rens Kamphorst, Jasper Ford, Gabrie M.H. Meesters, J Ruud Van Ommen*

1:50 Paper 135e: A Numerical and Experimental Investigation of a High Temperature Fluidized Bed for Thermal Energy Transfer — ***Krutika Appaswamy**, Jason Schirck, Zhiwen Ma, Aaron Morris*

2:10 Paper 135f: Analyzing Fluidized Bed Prediction Accuracy: From Modeling Framework to Material Properties — ***Casey LaMarche**, Jia Wei Chew, Raymond Cocco*

2:30 Paper 135g: On the Behaviour of Highly Volatile Feedstocks in Fluidised Bed Reactors during Advanced Thermochemical Conversions — ***Stefano Iannello***

(136) Nanostructured Materials for Pharmaceutical Applications

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, W-106A

Timothy Brenza, Chair

Sponsored by: Nanoparticles

12:30 Paper 136a: Toxicity of Orally Administered Magnetic Imaging Nanoprobes in an Inflammatory Intestinal Epithelial Cell Model — ***Shno Asad**, Christel A.S. Bergström, Alexandra Teleki*

12:48 Paper 136b: Making Nanostructured Materials for Health Applications Using Atomic Layer Deposition — ***J Ruud Van Ommen**, Volkert van Steijn, Antonia G. Denkova, Alina Rwei*

1:06 Paper 136c: Rational Design and Interspecies Translation of Glucose-Responsive Insulins and Insulin Delivery Systems By Computational Modeling — ***Sungyun Yang**, Jing Fan Yang, Xun Gong, Michael Strano*

1:24 Paper 136d: Processing of Lipid Nanoparticles for RNA Encapsulation — ***Navid Bizmark**, Satya Nayagam, Dawei Zhang, Sujit Datta, Rodney Priestley, Robert K. Prud'homme*

1:42 Paper 136e: Tailoring Spions through Polymer Coating Modifications for Cell Labeling and Tracking with Magnetic Particle Imaging (MPI) — ***Hayden Good**, Rita Das Mahapatra, Sitong Liu, Carlos Rinaldi-Ramos*

2:00 Paper 136f: Preparation of Low-Density Cannabidiol-Loaded Nanoparticles and Development of an *in Vitro* Release Assay — ***Nicholas Caggiano**, Brian K. Wilson, Rodney Priestley, Robert K. Prud'homme*

2:18 Paper 136g: Toxicity Studies of Chiral Nanoparticles *in Vitro* for Medical Applications — ***Macayla Caso**, Michael G. Benton, Kevin McPeak*

(137) Particulate Systems: Dynamics and Modeling: Applications

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, W-106B

Sarah Mena, Chair
Kelly Krzysik, Co-Chair

Sponsored by: Solids Flow, Handling and Processing

12:30 Paper 137a: Demonstration of Multi-Level Coarse-Grain (MCG) DEM Simulation Technique for Twin Screw Feeder — *Tarun De, Lokeshwar Mahto, **Jayanta Chakraborty**, Jitendra Kumar, Anurag Tripathi, William Ketterhagen, Maitraye Sen*

12:48 Paper 137b: CFD-DEM Simulations of Pinning for Gas-Solid Flows — ***Kanjakha Pal**, Yi Fan, Jorg Theuerkauf, Jonathan Lunn, John Holderness*

1:06 Paper 137c: Enhanced Flowability of Dense Bi-Disperse Granular Avalanche: The Role of Fine Grains — *Chongqiang Zhu, Ilaria Rucco, Fabio Dioguardi, **Raffaella Ocone***

1:24: Break

1:42 Paper 137e: Modelling Pneumatic Hopper Discharge of a Fine Bulk Solid Using a Coupled CFD-DEM Approach — *Stefan Pantaleev, Ravi Teja Chaganti, Dongil Chang, Hjalte Trnka, Tue Hansen, Thomas Kvistgaard Vilhelmsen, **Ioannis Fragkopoulos***

2:00 Paper 137f: Investigation of Particle Characteristics Influence of Crumbler® Rotary Shear Comminuted Granular Biomass on the Performance of Screw Feeding: Modeling and Experiment — ***Ahmed Hamed**, Yidong Xia, Nepu Saha, Jordan Klinger, David Lanning, Jim Dooley*

2:18 Paper 137g: Discrete Element Modeling of Wedge Hopper Discharge of Loblolly Pine Chips — ***Qiushi Chen**, Feiyang Chen, Yidong Xia*

2:36 Paper 137h: The Elastoplastic Flexural Behavior of Corn Stalks: An Experiment-Informed DEM Model and Process Simulation of a Knife Mill — ***Yidong Xia**, Jordan Klinger, Tiasha Bhattacharjee, John E. Aston, Vicki Thompson*

(138) Control Strategies in Pharmaceutical Development and Manufacturing I

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-122C

Shujauddin Changi, Chair
Christopher Marton, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

12:30 Paper 138a: Development of an Adsorbent Treatment Workflow for Impurity Removal — ***Zhenshu Wang**, Saurin Hiren Rawal, PhD, Jeremy Merritt, Daniel J. Jarmer*

12:51 Paper 138b: Development and Control of a Late-Stage API Crystallization Via Kinetics Modeling and Controlled Crystallization — ***Shujauddin Changi**, Berenice Lewandowski, Satyarit Rao, Billie Kline, David Willcox*

1:12 Paper 138c: Control of Ritter Side Products Via Reaction Engineering and Kinetic Modeling to Enable Robust Scale-up — ***Jennifer Lott**, Antonio C. Ferretti, Geoffrey E. Purdum, Antonio Ramirez, Scott Bader, Hon-Wah Man, Gerald Artman*

1:33 Paper 138d: Wet Milling of Mefenamic Acid for Seed Generation: Model-Driven Size Reduction for Maximizing Yield — ***Bhavik Mehta, PhD**, Cameron Brown, Niall Mitchell, Sara Ottoboni*

1:54 Paper 138e: Process Development and Characterization of an Acutely Hazardous Reaction through Data Rich Experimentation — ***Taylor Behre**, Ben W. H. Turnbull, Erin McCarthy, Nelo R. Rivera, Alexei Kalinin, Brittany Armstrong, Ji Qi, Andrew Solovyov, Jonathan McMullen*

2:15 Paper 138g: A Surrogate-Based Multi-Objective Optimization with Adaptive Sampling for Advanced Pharmaceutical Manufacturing — ***Yingjie Chen**, Marianthi Ierapetritou*

(139) Enabling Technologies: Progress in Tools and Technologies

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-123

Carla Luciani, Chair
Paridhi Agrawal, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

12:30 Paper 139a: Development of a Single-Tablet-Scale Direct Compression Process for the on-Demand Production of Personalized Tablets — ***Andreas Kottlan**, Andrea Zirkl, Jakob Geistlinger, Jörg Prassl, Johannes Obersriebnig, Benjamin Glasser, Johannes G. Khinast*

12:51 Paper 139b: On the Applications of Pervaporation in the Pharmaceutical Industry — ***Akshay Korde**, Sharad Maheshwari, Manish Kelkar, Shashank Shekhar, Ryan Ellis, Moussa Boukerche, Sarah Co, Eric Moschetta, Harsit Patel, Nandkishor Nere*

1:12 Paper 139c: Designing Rules for Continuous Separation of Enantiomers By Orthogonal Electrochromatography — ***Michal Pribyl***

1:33 Paper 139d: Thermal Analysis of the Wet Stirred Media Milling Process Used for the Production of Drug Nanoparticle Suspensions — ***Gulenay Guner**, Natasha Seetharaman, Sherif Elashri, Mirsad Mehaj, Ecevit Bilgili*

1:54 Paper 139e: Magnetophoretic Solid-Solid Separation of β-Lactam Antibiotics from Biocatalyst on a Pilot Plant Scale — ***Colton Lagerman**, Grant Marshall, Matthew McDonald, Martha Grover, Ronald Rousseau, Andreas Bommarius*

2:15 Paper 139f: Innovative Manufacturing Strategy Enabling Filament-Based 3D-Printing of Lipid-Based Advanced Dosage Forms — ***Moaaz Abdelhamid, MSc**, Carolina Corzo, Martin Spörk, Ioannis Koutsamanis, Carolina Alva, Ana Belén Ocampo, Mira Maisriemler, Eyke Slama, Dirk Lochmann, Sebastian Reyer, Tanja Freichel, Sharareh Salar-Behzadi*

2:36 Paper 139g: Ethylene Vinyl Acetate – How to 3D-Print Personalized Implantable Drug Delivery Systems — *Simone Eder, Lisa Kuchler, Eva Roblegg, Matthias Katschnig, **Martin Spörk***

(140) Physical Properties for Chemical Product and Process Design

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-222C

Kenneth Cox, Chair
Richard Elliot, Co-Chair

Sponsored by: Product Design

12:30 Paper 140a: Analysis of Vapor Pressures Using Family Variations: A Case Study of Hexadecanol Isomers — ***Paul Mathias**, Martin Schiller*

12:55 Paper 140b: Using Atom Modules and Modularity of Molecules for Property Prediction — ***Elias Martinez Hernandez**, Aburto Jorge*

1:20 Paper 140c: *Microstructural and Transport Properties of Graphene Polyacetylene Mixed Electron-Ion Conducting Films* — ***Benjamin Edward Slenker**, Aswin Prathap Pitchiya, Sitaraman Krishnan*

1:45 Paper 140d: Impact of Physical Properties on the Inhibition Effect of Green Corrosion Inhibitor Mixture Toward the Corrosion of Carbon Steel in the Acidic and Salty Solution — ***Tianxing Cai***

2:10 Paper 140e: Data-Driven Modeling to Predict the Physical Properties of the Lubricant — ***Chonghyo Joo**, Hyundo Park, Jongkoo Lim, Hyungtae Cho, Junghwan Kim*

(141) Process Development: Design, Risk Reduction, Implementation and Operations

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-221C

Michael Telgenhoff, Chair
Robert Nunley, Co-Chair
Deboleena Chakraborty, Co-Chair

Sponsored by: Technology Transfer and Manufacturing

12:30 Paper 141b: Lessons Learned from De-Risking the Production of Fuel Intermediates from Forest Residues — ***Sampath Gunukula**, Clayton Wheeler, Hemant P. Pendse*

12:55 Paper 141d: Solid-State Shear Pulverization (SSSP): An Investigation into Thermoplastic Types and Properties — ***Tyler Will**, Yiran Lu, Katsuyuki Wakabayashi*

1:20 Paper 141e: Addition Polymerization Case Study: Process Design and Scale-up at Multiple Sites — ***Roque Gochez Campos***

1:55 Paper 141f: Design and Analysis of Processes for Methane to Hydrogen Conversion Using the Piston Reactor Technology: A Comparative Analysis — ***Mary Katebah**, Aya Abousrafa, Mamoun Al-Rawashdeh, Patrick Linke*

(142) Regenerative Engineering Society II

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-121A

Karl Lewis, Chair
Paulos Mengsteab, Co-Chair

Sponsored by: Regenerative Engineering Society

12:30 Paper 142a: Making a new limb out of old cells: insights from limb regeneration in the Mexican Axolotl — ***Catherine McCusker***

1:05 Paper 142b: Delivering Bioactive Lipids from Synthetic Hydrogels as Regenerative Immunotherapy — ***Edward Botchwey***

1:40 Paper 142c: Musculoskeletal Modeling and Characterization of Lower Extremity Biomechanics in Response to an Engineered Post-ACL Reconstruction Treatment Protocol — ***Kristin Morgan***

2:15 Paper 142d: Leveraging biomaterial systems to address TBI via regenerative medicine — ***Sarah Stabenfeldt***

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(143) Adsorbent Materials for Sustainable Energy and Chemicals

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-131B

Federico Brandani, Chair
Youssef Belmabkhout, Co-Chair

Sponsored by: Adsorption and Ion Exchange

12:30 Paper 143a: Zeolite-13X- and ZIF-8 Filled PVA Mixed Matrix Membranes for Use in CO_2/N_2 and CO_2/CH_4 Separation — *Iris Samputu,* ***F Handan Tezel***

12:46 Paper 143b: Kinetic Process Assessment of H_2 Purification over Highly Porous Carbon Sorbents Under Multicomponent Feed Conditions — *Qasim Al-Naddaf, Shane Lawson, Ali Rownaghi,* ***Fateme Rezaei***

1:02 Paper 143c: Tuning Shape and Position of Step-Shaped Isotherms of Flexible MOFs through Ligand Functionalization for Improved CO_2/CH_4 Separation — ***Lukas Bingel****, Krista Walton*

1:18: Break

1:34 Paper 143e: MgO-CuO-CeO_x Sorbent Bead for a Trace Carbon Monoxide Removal for Fuel-Cell Grade Hydrogen Production — ***Gina Bang****, Seong-min Jin, Kyung-Min Kim, Chang-Ha Lee*

1:50 Paper 143f: Novel Adsorbent Design for Energy-Efficient and Economical Lithium Recovery from Unconventional Resources — *Hoon Choi, Marisa Moss, Elizabeth Kolbe, Stefan Haugen, Zbyslaw Owczarczyk, Bryan S. Pivovar,* ***Eric Karp***

2:06 Paper 143g: Development of Double-Functionalized Halloysite Nanotubes with Improved Adsorption Capacity for Carbon Capture — ***Oluwole Ajumobi****, Azeem Farinmade, Julia A. Valla, Vijay T. John*

2:22 Paper 143h: Amine Functionalization of Hyper-Cross-Linked Polymer (HCPs) for CO_2 Separation from Biogas — ***Olusola Johnson****, Babu Joseph, John Kuhn*

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(144) Adsorption Applications for Sustainable Energy and Chemicals

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-132A

Marcus Mello, Chair
Dipendu Saha, Co-Chair

Sponsored by: Adsorption and Ion Exchange

12:30 Paper 144a: Molecular Simulation and Experimental Study for the Separation of Azeotropic Hydrofluorocarbon Refrigerant Mixtures Using Silicalite. — ***Eliseo Marin Rimoldi****, Andrew Yancey, Edward Maginn, Mark B. Shiflett*

12:46 Paper 144b: Separation and Purification of High Value Chemicals Extracted from Food Waste — ***Yagya Gupta****, Laura Elizabeth Beckett, Sunitha Sadula, Vibin Vargheese, LaShanda Korley, Dionisios Vlachos*

1:02 Paper 144c: Microwave Swing Adsorption for Rapid Cycle CO2 Capture: Effect of Material and Process Parameters — *Yamid Alí Gómez Rueda, Eduardo Pérez-Botella, Brieuc Verougstraete, Mohsen Gholami,* ***Joeri Denayer***

1:18: Break

1:34 Paper 144e: Investigation of Hydrothermal Carbonization and Chemical Activation Process Conditions on Hydrogen Storage in Loblolly Pine-Derived Superactivated Hydrochars — ***Al Ibtida Sultana****, Toufiq Reza*

1:50 Paper 144f: Effect of Moisture on Sub-Ambient DAC with MIL-101(Cr)-Amine Sorbents — ***Guanhe Rim****, Mingyu Song, Pranjali Priyadarshini, Fanhe Kong, Ryan P. Lively, Christopher W. Jones*

2:06 Paper 144g: Impact of Functional Groups on LiCl Impregnation and Performance of LiCl@ MIL-101 Analogs for Atmospheric Water Harvesting — ***Mengjiao Wu***

2:22 Paper 144h: Application of ZIF-8 and Zeolite Y in a Pressure-Temperature Swing Adsorption Process for Simultaneous H_2 Purification and CO_2 Capture — ***Hassan Azzan****, David Danaci, Camille Petit, Ronny Pini*

2:38 Paper 144i: Adsorption of Pfas in Heteroatom-Doped Mesoporous Carbons: Experiment and Simulation — ***Dipendu Saha****, Zachary Romisher, Scott Van Bramer, Sandip Khan, Swasti Medha, Joanna Weyrich*

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(145) Distillation and Absorption Processes Fundamentals, Developments, Optimization, and Applications

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-225A

Tony Cai, Chair
Greg Cantley, Co-Chair
Andrew Sloley, Co-Chair

Sponsored by: Distillation and Absorption

12:30 Paper 145a: Optimization of the Vapor Flow Distribution in a Distillation Column Using Computational Fluid Dynamics — ***Yu Feng****, Tony Cai*

12:55 Paper 145b: Gravity Flow and Internal Piping in Distillation Columns – the Devil Is in the Details — ***Andrew Sloley***

1:20 Paper 145c: Quantifying the Effect of Stripping Factor on Tray Column Efficiency Under Non-Total Reflux Conditions — ***Rukhsar Ahmed****, Tony Cai, Kenneth McCarley, Sayeed Mohammad, Michael Miranda, Clint Aichele*

1:45 Paper 145d: Optimal Design and Operation of Ternary Hybrid Dividing Wall Columns — *Dian Ning Chia, Fanyi Duanmu,* ***Eva Sorensen***

2:10 Paper 145e: Performances of Advanced Structured Packings Produced By 3D Foam Printing for Gas-Liquid Multiphase Contactors in FGD Process Intensification — ***Domenico Flagiello****, Daniele Tammaro, Alessandro Erto, Pierluca Maffettone, Amedeo Lancia, Francesco Di Natale*

2:35 Paper 145f: Relaxing the Constant Relative Volatilities and Constant Molar Overflow Assumptions in Distillation While Retaining Their Benefits — ***Tony Joseph Mathew****, Mohit Tawarmalani, Rakesh Agrawal*

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(146) Fluid Particle Separations in Energy and Environmental Systems

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-131C

Jenifer Gomez Pastora, Chair
Oluwaseyi Odueyungbo, Co-Chair

Sponsored by: Fluid-Particle Separations

12:30: Break

12:55 Paper 146b: Enhanced Diffusiophoretic Mobility and Removal of Colloidal Water Contaminants By Tunable CO_2 Flux — ***Esai Lopez****, Patryck Michalik, Shicheng Lyu, Alex D. Paulsen, Elizabeth Stewart, Andrew R Teixeira*

1:20 Paper 146c: Thermodynamic Modeling of Mineral Solubility in High-Temperature, High-Pressure Petroleum Systems. — ***Isaac Gamwo****, Derek Hall, Serguei Lvov, Hseen Baled*

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(147) Frontiers in New Materials and Membranes for Bioseparations

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-130

Cristiana Boi, Chair
Raja Ghosh, Co-Chair

Sponsored by: Bio Separations

12:30 Paper 147a: New Design for Hollow Fiber Membrane Module: Feasibility Study Based on Computational Fluid Dynamic Simulations — *Yating Xu,* ***Raja Ghosh***

12:50 Paper 147b: Nature Inspired Convective Chromatography Columns for Preparative Separations — *Riccardo Onesti, **Cristiana Boi***

1:10 Paper 147c: A Comparative Study of Protein a Membranes for the Rapid Purification of Monoclonal Antibodies — ***Joshua Osuofa**, Scott Husson*

1:30 Paper 147d: Purification of Biotherapeutics By High-Productivity Nonwoven Based Membrane Adsorbers — ***Jinxin Fan**, Ruben Carbonell, Cristiana Boi*

1:50 Paper 147e: Membrane Adsorbers to Capture Cu from Mixed Metal Acidic Solutions in Support of Radiopharmaceuticals — ***Maura Sepesy**, Benjamin Fugate, Joelle Scott, Alec Johnson, Christine Duval*

2:10 Paper 147f: Novel Adsorptive Membranes for mRNA Capture for Vaccine Manufacture — ***Riddhi Banik**, Thomas Neumann, Mirco Sorci, Miral Al Sharabati, Zerui Hao, Manasa Chillara, Weibo Zhao, Todd Przybycien, James (Chip) Kilduff, Georges Belfort*

2:30 Paper 147g: Demonstrating Mathematical Equivalence between Partial Least Squares and the Beer-Lambert Law in Estimating Protein Concentrations with Spectroscopic Data — ***Claire Velikonja**, Ian Gough, Brandon Corbett, David Latulippe, Prashant Mhaskar*

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(148) Modeling and Control of Crystallization

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-131A

Giovanni Maria Maggioni, Chair
Ryan Snyder, Co-Chair
Xiaobin Jiang, Co-Chair

Sponsored by: Crystallization and Evaporation

12:30: Introductory Remarks

12:33 Paper 148b: Developing a Novel Size-Dependent Growth Modeling Method for the Batch Crystallization of Carbamazepine from Variable Seed Crystal Size Distributions — ***Harrison Kraus**, David A. Acevedo, Thomas O'Connor, Dongxia Liu, Adil Mohammad*

1:02 Paper 148c: Digital Design of Crystallization Process: Application of a Mechanistic Morphological Crystallizer Model to Improve Powder Flowability Via Aspect Ratio Reduction — ***Niall Mitchell**, Efty Hadjittofis, Filipe Calado, Sélim Douieb, Ugo Cocchini, Jan-Sebastiaan Uyttersprot, Jerome Mantanus, Nicolas Carly*

1:31 Paper : Scale-up of a Yield-Stress Slurry of Needle-like Crystals Using the Cavern Model — ***Paul Larsen***

2:00 Paper 148d: Process Intensification for Continuous Manufacturing of Energetic Materials Via Model-Free Quality-By-Control Direct Design and Model-Based Digital Design Approaches — ***Montgomery Smith**, Monika Neal, Daniel Laky, Wei-Lee Wu, Jaron Mackey, Zoltan Nagy*

2:29 Paper 148e: Design of the Cooling Crystallization Process Using the Machine Learning-Based Strategy — ***Yiming Ma***

2:58: Concluding Remarks

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(149) Novel Approaches to CO_2 Utilization I

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-226C

Gregory Kline, Chair
Damilola Daramola, Co-Chair
Joseph Stoffa, Co-Chair

Sponsored by: Sustainable Energy

12:30 Paper 149a: Sustainable Processing of Composite Materials — ***Daniel Kopp**, Paniz Foroughi, Paul Antonick, Noemie Denis, Richard E. Riman*

12:45 Paper 149b: CO_2 As a Carbon Source in Direct Synthesis of Dimethyl Ether from Syngas over Silicotungstic Acid Incorporated Bifunctional Catalysts — *Birce P. Karaman, Nuray Oktar, Gulsen Dogu, **Timur Dogu***

1:00 Paper 149c: Direct Hydrogenative Conversion of CO_2 to Liquid Hydrocarbons Using Tandem Heterogeneous Catalyst — ***Yongseok Kim**, Kyungsu Na*

1:15 Paper 149d: Mine Tailings for CO2 Mineralization - Towards Efficient Processes and Usable Products — ***Andreas Voigt**, Kai Sundmacher*

1:30 Paper 149e: Life Cycle Analysis Tools to Determine Environmental Footprint of Carbon Utilization Projects — ***Sheikh Moni**, Michelle Krynock, Timothy Skone*

1:45 Paper 149f: Synergistic Effect of Zn_2GeO_4 nanorod Decorated Metal Organic Framework ZIF-67 for Enhanced Photo Catalytic CO_2 Reduction to Methanol Under Visible Light Irradiation — ***Amar Nath Samanta***

2:00 Paper 149g: Cooperative Bifunctional Adsorbent/Catalyst Structured Monoliths for Direct Capture-Utilization of CO_2 with Cogeneration of Ethylene and Propylene — ***Khaled Baamran**, Shane Lawson, Fateme Rezaei, **Ali Rownaghi***

2:15 Paper 149h: Intensification of CO2 Utilization in Membrane Reactors — ***Michael Patrascu***

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(150) Sustainable Biorefineries Plenary Session (Invited Talks)

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-226B

Ramalingam Subramaniam, Co-Chair
Eric Tan, Co-Chair
Ana I. Torres, Co-Chair

Sponsored by: Sustainable Biorefineries

12:30 Paper 150a: Rethinking Cellulosic Biofuels: Toward a Depot-Enabled, Nuclear-Assisted Biorefinery System — ***Bruce Dale**, Charles Forsberg*

1:10 Paper 150b: The Role of Biomass in Cross-Sector Decarbonization — ***Andrea Bailey***

1:50 Paper 150c: Sustainable Aviation Fuels from Sunlight and Air — ***Aldo Steinfeld***

2:30 Paper 150d: Chemical and Physical Process Applications in Environmental Engineering... Towards a Sustainable Environment — ***Emilio Nehme***

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(151) Sustainable Management and Uses of Post-Consumer Materials and Waste

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-226A

Jason Trembly, Chair
Gerardo Ruiz-Mercado, Co-Chair
Damilola Daramola, Co-Chair

Sponsored by: Sustainability Science and Engineering

12:30 Paper 151a: Rare Earth Element Recovery from e-Waste: A Techno-Economic Analysis (TEA) and Life Cycle Analysis (LCA) Case Study of Terfenol-D Scrap Recycling — ***Esther Sanchez Moran**, Mark Mba Wright, Dan Bina, Denis Prodius, Ikenna C. Nlebedim*

12:45 Paper 151b: Tracking Industrial Wastewater Transfers to Publicly Owned Treatment Works, a Data Engineering Approach — ***David Perez**, Gerardo Ruiz-Mercado*

1:00 Paper 151c: Optimization of the Solvent-Targeted Recovery and Precipitation (STRAP) Process for Multilayer Plastic Recycling — ***Aurora Del Carmen Munguia Lopez**, Yue Shao, Victor Zavala*

1:15 Paper 151d: Hydrometallurgical Recycling of Valuable Materials from Lithium-Ion Battery Scrap; A Process Route — ***Rafaela Greil**, Georg Rudelstorfer, Susanne Lux*

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(152) Applications of Data Science in Molecular Sciences I

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-230

Johannes Hachmann, Chair
Connor Coley, Co-Chair
Qing Zhao, Co-Chair

Sponsored by: Applications of Data Science to Molecules and Materials

12:30 Paper 152a: Combining functional group and Graph Neural Networks Towards Interpretable Molecular Property Models — ***Adem Rosenkvist Nielsen Aouichaoui***, *Fan Fan, Seyed Soheil Mansouri, Jens Abildskov, Gurkan Sin*

12:45 Paper 152b: Evaluation of Sampling Algorithms to Explore the Latent Space Created By Deep Generative Models — ***Fangxi Wang***, *Parisa Farzeen, Charles Plate, Lakshmikumar Kunche, Sanket Deshmukh*

1:00 Paper 152c: Automatic Creation of Molecular Substructure Descriptors for Estimation of Pure Compound Properties — ***Qiong Pan***, *Jie Li, Xiaolei Fan*

1:15 Paper 152d: *Data-Driven Chemical Property Models for Energetic Materials Using Transfer Learning* — ***Joshua Lansford***, *Brian C. Barnes, Betsy Rice, Klavs Jensen*

1:30 Paper 152e: Machine-Learning a Solution for Reactive Simulations of Complex Chemical Systems — ***Rebecca Lindsey***, *Laurence E. Fried, Nir Goldman, C. Huy Pham, Sorin Bastea*

1:45 Paper 152f: Capturing Molecular Interactions in Graph Neural Networks: A Case Study in Multi-Component Phase Equilibrium — ***Shiyi Qin***, *Shengli Jiang, Prasanna Balaprakash, Reid Van Lehn, Victor Zavala*

2:00 Paper 152g: A Statistical Analysis of Computational Hydrogen Bond Features in Hydrophobic Non-Ion Deep Eutectic Solvents and Non-Deep Eutectic Solvents — ***Usman Abbas***, *Joseph Tapia, Yuxuan Zhang, Mohammad Selim, Jian Shi, Jin Chen, Qing Shao*

2:15 Paper 152h: Predicting Temperature-Dependent Activity Coefficients of Ionic Liquid-Solute Systems through Graph-Based Machine Learning — ***Jan G. Rittig***, *Karim Ben Hicham, Artur M. Schweidtmann, Manuel Dahmen, Alexander Mitsos*

2:30 Paper 152i: Property Prediction of Amine-Functionalized Ionic Liquids for Multi-Scale Carbon Capture Design and Optimization — ***Austin Keller***, *Pratik Kelkar, Michael Baldea, Mark Stadtherr, Joan Brennecke*

2:45 Paper 152j: Machine-Learning Enabled Screening of MOFs for Ion Selective Membranes — ***Shuwen Yue***, *Aditya Nandy, Heather Kulik*

(153) Chemical Engineering Principles Advancing Medicine I

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-126C

Elizabeth Nance, Chair
Huanan Zhang, Co-Chair

Sponsored by: Chemical Engineers in Medicine

12:30 Paper 153a: Slow-Release Nanoparticles for Chronic Pain Management — ***Parker Lewis***, *Rachel Pollard, Rocco Latorre, Dane Jensen, Brian Schmidt, Nigel Bunnett, Nathalie M. Pinkerton*

12:51 Paper 153b: *Pseudomonas Aeruginosa* Reverse Diauxie Is a Multidimensional, Optimized, Resource Utilization Strategy Facilitating Chronic Wound Colonization — *S. Lee McGill, Yeni Yung, Kristopher A. Hunt, Michael Henson, Luke Hanley,* ***Ross P. Carlson***

1:12: Break

1:33 Paper 153d: Evaluating Antimicrobial Drug Formulations on a 3D Biofilm Growth Model Under Simulated *In Vivo* Conditions — ***Yadiel Varela-Soler***, *Himani Chavda, Swarnima Roychowdhury, Veronica Farag, Patrick Erickson, Biju Parekkadan, Charles Roth*

1:54: Break

2:15 Paper 153f: Improving Therapeutic Protein Secretion in Probiotic Yeast *Saccharomyces Boulardii* using a Multifactorial Engineering Approach. — ***Deniz Durmusoglu***, *Ibrahim Al'Abri, José Luis Martinez Ruiz, Nathan Crook*

2:36 Paper 153g: A Low-Cost Strategy for Genotypic Antimicrobial Resistance Detection Using Oligonucleotide Ligation Assay — ***Ayushi Chauhan***, *Bhushan Toley*

(154) Machine Learning in Materials Discovery

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-227A

John Ekerdt, Chair
Jane Chang, Co-Chair

Sponsored by: Material Interfaces as Energy Solutions

12:30 Paper 154a: Data-Driven Protein Design — ***Andrew Ferguson***

12:56 Paper 154b: Low-Dimensional Fluctuating Interfaces for Efficient Separations — ***Narayana Aluru***

1:22 Paper 154c: Enabling Catalyst Discovery through High-Throughput Experimentation and Machine Learning — ***Jochen Lauterbach***

1:48 Paper 154d: Predicting the Transition Temperature of Multi-Responsive Poly(N-isopropylacrylamide)-Based Microgels Using a Cluster-Based Partial Least Squares Modelling Approach — ***Seyed Saeid Tayebi***, *Prashant Mhaskar, Todd R. Hoare*

2:04 Paper 154e: Designing Metamorphic Materials with a Machine-Learning Guided Genetic Algorithm — ***Kuan-Lin Chen***, *Rebecca Schulman*

2:20 Paper 154f: Establishing Structure-Function Relationships in Low-Dimensional Mxenes Using Machine Learning — ***Tej Choksi***, *Pranav Roy, Lavie Rekhi, Hong Li, See Wee Koh*

2:36 Paper 154g: High Strength Polymer Composites Design for Lightweight Vehicles Via Stacked Transfer Learning and Explainable Artificial Intelligence — ***Jaewook Lee***, *En Sup Yoon, Dongil Shin*

(155) 3D Printing Novel Methods and Applications

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-221B

Blair Brettmann, Chair
William Phillip, Co-Chair

Sponsored by: 3D Printing

12:30 Paper 155a: "Autonomous 3D Printing" for Novel Food and Pharmaceutical Applications — ***Anson W. K. Ma***, *Ethan Chadwick, Christopher Maiorana, Maryam Pardakhti, Shing-Yun Chang, Mingyang Tan, Pouria Hoveida, Guoan Zheng, Yushuo Niu, Qian Yang*

12:50 Paper 155b: Achieving High Optical Translucency in SLA-Printed Elastic Materials for Patient-Specific Anatomical Models in Cardiovascular Medicine Applications — ***Alan Aguirre-Soto***

1:10: Break

1:30 Paper 155d: Understanding Multiphase Behavior of Additively Manufactured Lattices: Progress Towards Personalized Biomedical Tools and Platforms — ***Ian Woodward***, *Yinkui Yu, Emily Kolewe, Catherine Fromen*

1:50 Paper 155e: Masked Stereolithography Printing for Rapid Prototyping of Microfluidic Systems with Embedded Functional Components — ***Isteaque Ahmed***, *Aashish Priye*

2:10 Paper 155f: Novel Tool for Evaluating Powder Feedstock Suitability for AM Spreading Processes — *Tony Thornton,* ***Amalia Thomas***, *Jamie Clayton, Dan Oropeza*

(156) Applied Artificial Intelligence, Big Data, and Data Analytics Methods for Next-Gen Manufacturing Efficiency II

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-221A

Joel Paulson, Chair
Ahmad Arabi Shamsabadi, Co-Chair
Mona Bavarian, Co-Chair

Sponsored by: Next-Gen Manufacturing

12:30 Paper 156a: Keynote Talk-Bayesian Optimization for Additive Manufacturing of Thermoelectric Materials and Devices — ***Alexander Dowling***, *Ke Wang, Mortaza Saeidijavash, Minxiang Zeng, Tengfei Luo, Yanliang Zhang*

1:00 Paper 91a: Probabilistic Machine Learning Based Soft-Sensors for Product Quality Prediction in Batch Processes — ***Max Mowbray***, *Philip Martin, Dongda Zhang*

1:20: Discussion

1:30 Paper 156c: Application of Artificial Intelligence to Predict Surfactant Adsorption — ***Shams Kalam***, *Sidqi Abu-Khamsin, Muhammad Shahzad Kamal, Shirish Patil, Syed Hussain, Emad W. Al Shalabi*

1:48 Paper 156d: A Deep-Learning Model of a Crude Distillation Unit — ***Jiannan Zhu***, *Feng Qian, Chen Fan, Vladimir Mahalec*

2:06 Paper 156e: The Effect of Chemical Representation on Active Machine Learning Towards Closed-Loop Optimization — ***Alexander Pomberger***

2:24 Paper 156f: Neural Network-Based Automated Detection of Functional Groups in Spectroscopic Data- Bridging the Gap in Online Monitoring of Complex Reaction Systems — ***Karthik Srinivasan***, *Vinay Prasad*

2:42 Paper 156g: Effects of Noise When Implementing Linear Control Laws on Quantum Computers — ***Keshav Kasturi Rangan***, *Kip Nieman, Helen Durand*

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(157) Student Competition in Sensors (Sponsored)

Monday, Nov 14, 12:30 PM
Phoenix Convention Center, N-231A

Qingshan Wei, Chair
Han-Sheng Chuang, Co-Chair

Sponsored by: Sensors for Sustainability

12:30 Paper 157a: Introduction to Session — ***Qingshan Wei***

12:40 Paper 157b: A Low-Cost and Facile Color-Changing Nanofilm for Temperature Monitoring and Recording — ***Md Nayeem Hasan Kashem***, *Wei Li*

1:00 Paper 157c: Using Molecular Dynamics Simulations to Model Entropic Changes upon Peptide Binding — ***Jazmine Torres***, *Ryan Peterson, Christopher Kieslich, Robert Pantazes*

1:20 Paper 157d: A Capacitive Electronic Tongue Based on Cyclodextrins for Rapid Assessment of Sepsis Biomarkers — ***Zahra Panahi***, *Jeffrey Halpern*

1:40 Paper 157e: Nonfluorescent CRISPR-Cas12a Biosensor By Sizing λ DNA — ***Noor Mohammad***, *Shrinivas Siddhivinayak Katkam, Qingshan Wei*

2:00 Paper 157f: Point-of-Use Fiber-Based Haloacetic Acid Sensor for Water at Sub-USEPA Regulation Limits — ***Hadi Rouhi***, *Colton Duprey, Elham Ghalavand, Emily Linn, Sarah Veres, George Chen, Leigh Terry, Mark Elliott, Evan Wujcik*

2:20 Paper 157g: Electrochemical ELISA Biosensor for SARS-COV-2 Nucleocapsid Detection — ***Katherine Austin***, *Xingcheng Zhou, Ariel Furst*

2:40 Paper 157h: Gold Leaf Electrochemical Biosensors for Detection of Infectious Diseases — ***Joshua Chaj Ulloa***, *Marjon Zamani, Xingcheng Zhou, Ariel Furst*

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(158) Chemical Engineering Policy (WISE) Award Recipient Talks (Invited Talks)

Monday, Nov 14, 1:30 PM
Phoenix Convention Center, N-127A

Sponsored by: Public Affairs and Information Committee (PAIC)

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(159) The Langer Prize for Innovation and Entrepreneurial Excellence Award Presentation and Lecture

Monday, Nov 14, 1:45 PM
Phoenix Convention Center, North Ballroom 120D

Sponsored by: Awards Committee

1:45: Introductory Remarks

2:00: 2022 Prize Presentation

2:05: Invited Remarks

2:15 Paper 159a: 2022 Langer Fellow Presentation: "Developing novel microbial hosts for waste plastic upcycling" — ***Tae Seok Moon***

2:45: Concluding Remarks

2:50: Networking & Light Refreshments

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(160) Wilson Award Presentation and Lecture (Invited Talks)

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-224AB

James Laurinat, Chair
Maximilian Gorensek, Co-Chair

Sponsored by: Nuclear Engineering Division

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(161) Laboratory and Pilot Plant Safety

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-221C

Michael Trainor, Chair
Kakasaheb Nandiwale, Co-Chair

Sponsored by: Pilot Plants

3:30 Paper 161a: Application of Calorimetric Data in Reactive Chemicals Evaluations of Laboratory-Scale Processes — ***Jessica E. Nichols***

4:00 Paper 161b: Safety Issues with Installing Pilot Plants in Hoods and Ventilated Enclosures — ***Richard Palluzi***

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(162) Fluid Mechanics Poster Session

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, North Hall E

John Frostad, Co-Chair
Steve Kuei, Co-Chair

Sponsored by: Fluid Mechanics

Poster 162a: Influence of Surfactants, Polymers and Proteins on Foam Film Drainage — ***Carina Martinez***, *Lena Hassan, Chrystian Ochoa, Vivek Sharma*

Poster 162b: Acoustic Streaming Flows in Non-Newtonian Fluids: Numerical Simulations and Experiments — *Beijia Yao, Vijay K. Gupta, Cheng Wang,* ***Joontaek Park***

Poster 162c: Stability of a Radially Expanding Liquid Sheet in Presence of Gas Boundary Layer — ***Soumya Kedia***, *Puja Agarwala, Mahesh Tirumkudulu*

Poster 162d: Large Eddy Simulations (LES) to Capture Turbulence Modulation in Inertial Particle-Laden Turbulent Channel Flows — ***Partha Goswami***, *Naveen Rohilla, Pradeep Muramulla*

Poster 162e: A New Stress Model for Gas-Particle Flows from Dilute to Dense Regimes with Particle Friction and Volume Fraction Gradient — ***Junnan Zhao***, ***Guodong Liu***

Poster 162f: Rheology of Highly-Loaded Polymer-Ceramic Suspensions for Direct-Ink-Writing 3D Printing — ***Ria Corder***, *Arezoo Ardekani, Kendra A. Erk*

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(163) Poster Session: Interfacial Phenomena (Area 1C)

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, North Hall E

Christopher Wirth, Chair
Marina Tsianou, Co-Chair

Sponsored by: Interfacial Phenomena

Poster 163a: Improved Carbon Dioxide Hydrate Formation Using Superabsorbent Polymers (SAPs) and Tetrahydrofuran (THF) without Mechanical Agitation — ***Dong Woo Kang***, *Wonhyeong Lee, Yun-Ho Ahn, Jae Lee*

Poster 163c: Microscopic Diffusion of a Chemical Warfare Agent Simulant in the Presence of Water in Nafion Membranes By PFG NMR — ***Blake Trusty***, *Junchuan Fang, Anastasios Angelopoulos, Sergey Vasenkov*

Poster 163d: Significance of Π-Electrons in the Adsorption of Corrosion Inhibitors for Carbon Steel Rebars in Simulated Concrete Pore Solution — ***Ahmed Mohamed***, *Donald Visco Jr., David M. Bastidas*

Poster 163e: Influence of Secondary Heteroatoms within Aromatic Compounds on Corrosion Inhibition of Carbon Steel — ***Karl Breimaier***, *Ahmed Mohamed, Donald Visco Jr., David M. Bastidas*

Poster 163f: Development of Chemically Degradable Epoxy Resins for Upcycling Carbon Composites By Using Molecular Dynamics — ***Hyoje Son***, *Hyunseo Park, Sweety Verma, Pil Seung Chung*

Poster 163g: Bacterial Nanocellulose as an Eco-Friendly Additive in Water-Based Drilling Fluids Applied to Shale Formations — ***Diana Estenoz***, *María Laura Foresti*

Poster 163h: Confinement Induced Alteration of Morphologies of Oil-Water Emulsion — ***Animangsu Ghatak***

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(164) Poster Session: Bioengineering

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, North Hall E

Yongchan Kwon, Chair
Wheaton Schroeder, Co-Chair
Jason Boock, Co-Chair
Nicholas Sandoval, Co-Chair

Sponsored by: Bioengineering

Poster 664b: Sampling of Contact Lens Saline for Sars-Cov-2 Virus Detection Applications — ***Hazim Aljewari***, *Shadrach Ibinola, Kevin Clark, Vicki Thompson, Audie Thompson, Shannon Servoss, Robert Beitle*

Poster 164a: A Polyketide Synthase-Based Platform for Making Plastic Monomers of Polydiketoenamines — ***Zilong Wang***, *Seokjung Cheong, Robert W. Haushalter, Jay Keasling*

Poster 164c: Thermoacidophilic Archaea Enhance Bioleaching of Chalcopyrite for Copper Recovery — ***Mohamad Javad Haghighat Manesh***, *Dan Willard, April Lewis, Robert M. Kelly*

Poster 250b: Enzymatic Reactive Extraction of Fermentation Products for the Production of Short-Chain Esters — ***Danika Kartchner***, *Aditya Sarnaik, Dylan Ellis, Apurv Mhatre, Ryan Davis, Somnath Shinde, Arul Mozhy Varman*

Poster 164d: Engineering Human Mesenchymal Bodies for Exosome Secretion in a Novel 3-D Printed Microchannel Bioreactor. — *Richard Jeske,* ***Xingchi Chen***, *Logan Mulderrig, Wenhao Cheng, Changchun Zeng, Jingjiao Guan, Daniel T. Hallinan Jr., Yan Li*

Poster 164e: Leveraging Advances in Proteomics to Mathematically Model Cell Signaling Processes: A Case Study on TGFβ Signaling in Valve Interstitial Cells — ***Daniel P. Howsmon***, *Toni M. West, Michael S. Sacks*

Poster 164f: Amyloid Aggregation of Enzymes Under Non-Denaturing Conditions — *Timothy Charlton, Emre Erkanli,* ***Jin Ryoun Kim***

Poster 164g: Peptide Aggregation Induced Immunogenic Rupture (PAIIR) on Breast Cancer Spheroid Model — ***Gokhan Gunay***

Poster 164h: Systematic Evaluation of Protein-Small Molecule Conjugates on Yeast Surface — ***Manjie Huang***, *Abbigael Harthorn, Benjamin J. Hackel, James Van Deventer*

Poster 164i: Modulated Cell-Free Protein Synthesis System for Biomanufacturing of Multiple Disulfide Bond Containing Therapeutic Proteins — ***Claire Lanclos***, *Parker Hannan, Yongchan Kwon*

Poster 164j: Engineer Novel Functional Proteins in Plant Cell Culture for Industrial and Biomedical Applications — ***Jianfeng Xu***

Poster 164k: Acoustic Force Spectroscopy Enables Multiplexed Single-Molecule Characterization of Protein-Carbohydrate Binding — *Markus Hackl,* ***Shishir Chundawat***

Poster 164l: Designing Versatile Beta Roll Peptide Scaffolds — ***Matthew Lucia***, ***Devin Golla***, *Farid Khoury, Scott Banta*

Poster 164m: Thermostable Enzymes for Error Correction of DNA — ***Rushant Sabnis***, *Madeline Jordan, Paul de Figueiredo, Qing Sun*

Poster 164n: Exploring Structure-Function Relationships Governing Activity of the Cyanobacterial Bicarbonate Transporter Sbta — ***Sydney Parrish***, *Christopher Jones, Amanda Godar, David Nielsen, Brent L. Nannenga*

Poster 164o: A Novel Thiolase with Enhanced Activity of ATP-Independent Triacetic Acid Lactone (TAL) Production — ***Seokjung Cheong***, *Zilong Wang, Jose Henrique Pereira, Andy Degiovanni, Carolina Araujo Barcelos, Robert W. Haushalter, Paul D. Adams, Jay Keasling*

Poster 164p: Engineering Antibody Fusion Proteins for Targeted Intracellular Therapeutic Delivery — ***Kyle Kaeo***, *Seth Ludwig, Jamie Spangler*

Poster 164q: A Novel Thermophilic Enzyme for DNA Based Error Correction — ***Rushant Sabnis***, *Madeline Jordan, Paul de Figueiredo, Qing Sun*

Poster 164r: The Influence of Electrostatic Distribution on Small Molecule Binding of Coiled-Coil Protein Microfibers — ***Julia Monkovic***, *Dustin Britton, Sihan Jia, Chengliang Liu, Jin Kim Montclare*

Poster 164s: Synthesis and Evaluation of Megamolecule Dendrimers in Cancer Therapy — ***Blaise Kimmel***, *Milan Mrksich, John Wilson*

Poster 164t: Leveraging Synthetic Biology and Gut-on-a-Chip Systems to Investigate the Mechanistic Role of H_2S in the Gut — ***Justin Hayes***, *Benjamin Woolston, Ryan Koppes*

Poster 164u: Novel Magnetic Biosensor for COVID-19 Surveillance through Wastewater-Based Epidemiology — ***Stefano Ciannella***, *Sowrav Barua, Jenifer Gomez Pastora*

Poster 164w: Yeast Surface Display of Sars-Cov-2 Receptor Binding Domain (RBD) for Diagnostic Purposes — ***Shadrach Ibinola***, *Hazim Aljewari, Kaylin Hicks, Sebastian Freeman, Robert Beitle, Shannon Servoss, Kaiming Ye, Ahmed El Masheiti, Kevin Clark, Vicki Thompson, Beth Cobb*

Poster 164x: Engineering Ligand-Specific Biosensors for Aromatic Amino Acids, Neurochemicals, and Other Structurally Similar Compounds — ***Chenggang Xi***, *Austin Rottinghaus, Matthew Amrofell,* ***Tae Seok Moon***

Poster 164y: The Change of Magnetic Susceptibility of Red Blood Cells Depending on the Density. — ***Hyeon Choe***, *Mitchell Weigand, Xian Wu, Jacob Strayer, Jenifer Gomez Pastora, Jeffrey Chalmers*

Poster 164z: Identifying Key Biomarkers and Underlying Mechanisms behind Pediatric Influenza Infection — ***Lauren Luciani***, *Jason E. Shoemaker*

Poster 164aa: Human Forebrain Organoid-Derived Extracellular Vesicle Labelling with Iron Oxides for in Vitro Magnetic Resonance Imaging — ***Chang Liu***, *Mark Marzano, Shannon Helsper, Xingchi Chen, Laurie Muok, Changchun Zeng, Li Sun, Samuel C. Grant, Yan Li*

Poster 164ab: Red and White Blood Cell Magnetic Analysis and Separation: Potential for Hematologic Disease Diagnosis — ***Sowrav Barua***, *Stefano Ciannella, Jeffrey Chalmers, Jenifer Gomez Pastora*

Poster 164ac: Monitoring the Activity of Optogenetically Engineered Cardiomyocytes Using Microelectrode Arrays Chips — *Olurotimi A. Bolonduro,* ***Zijing Chen***, ***Emmanuel Tzanakakis***, *Brian P. Timko*

Poster 164ad: Characterization of Mneongreen in the Cell-Free Protein Synthesis System and Optimizations of Signal Output for Biosensor Application — ***Caroline Copeland***, *Jeehye Kim, Pearce Copeland, Chloe Heitmeier, Yongchan Kwon*

Poster 164ae: Biosensor Engineering for Reliable Production Detection — ***Jennifer Kaczmarek***, *Kristala Prather*

Poster 164af: Combining the Use of Predictive Modelling Tools and Experimental Data to Optimize Formulation Design for Novel Modalities in Biologics — ***Julia E. Vela Ramirez***, *Marco Blanco, Suzanne M. D'Addio, Heidi Ferguson, Suman Luthra*

Poster 164ag: Overexpression of Native Gene Presumably Encoding for D-Xylose Reductase in *Escherichia coli* leads to High Xylitol Production — ***Angelo Banares***, *Grace Nisola, Won-Keun Lee, Wook-Jin Chung*

Poster 164ah: Leveraging Propionate-Induced Growth Inhibition in *Corynebacterium Glutamicum* to Evolve Improved Methylmalonyl-CoA-Dependent Polyketide Synthases — ***Chunjun Zhan***, *Robert W. Haushalter, Jay Keasling*

Poster 164ai: Metabolic Engineering of Four Host Microbes for the Production of Green Leaf Volatiles and Precursor Molecules — ***Qingyun Dan***, *Jing Huang, Jay Keasling*

Poster 164aj: Introduction of Abiological Reactions into Biosynthesis — ***Jing Huang***, *Aindrila Mukhopadhyay, Jay Keasling*

Poster 164ak: Functional Characterization of paclitaxel Transporters in *Taxus Cuspidata* to Enhance Secretion — ***Md Tahsin Rahi***, *Cassandra Brzycki Newton, Alexandra Harrison, Lauren Revene, Susan Roberts*

Poster 164al: Characterizing a cAMP/Crp Mediated Metabolic Futile Cycle in Bacterial Persisters — ***Hanny Ngo***, *Sayed Golam Mohiuddin, Mehmet Orman*

Poster 164am: Environment Constrains Fitness Advantages of Division of Labor in Microbial Consortia Engineered for Metabolite Push or Pull Interactions — *Ashley Beck, Alissa Bleem, Martina Du, William Harcombe, Hans C. Bernstein, Jeff Heys, Tomas Gedeon,* ***Ross P. Carlson***

Poster 164an: Engineering *Y. Lipolytica* for the Biosynthesis of Geraniol — ***Ayushi Agrawal***, *Zhiliang Yang, Mark Blenner*

Poster 164ao: Understanding Strain Instability in Yarrowia Lipolytica — ***Philip Gitman***, *Alyssa M. Worland, Yinjie Tang, Mark Blenner*

Poster 164aq: Effect of Alternative Sigma Factors on Metabolic Activity in *E. coli* — ***Ryan Armstrong***, *Elizabeth Kornreich, Michael Anderson, Jason Boock*

Poster 164ar: Developing a Novel Microbial Host and Synthetic Biology Tools for Valorizing Waste Polyethylene Terephthalate and Lignin-Derived Compounds — ***Jinjin Diao***, ***Yifeng Hu***, ***Tae Seok Moon***

Poster 164as: Plastics Degradation By the Yellow Mealworm Gut Microbiota and Associated Enzyme Studies — ***Ross Klauer***, *Lummy Monteiro, Jyoti Singh, Kevin Solomon, Mark Blenner*

Poster 164at: Kinetic Rates and Image Based Single Cell Profiling for Characterizing Autophagy. — ***Nitin Sai Beesabathuni***

Poster 164au: Integrating Metabolomics and Fluxomics to Study Cancer Metabolism in Low Glucose Environments — ***Aliya Lakhani***

Poster 164av: Human Liver Diverticulum Triggers Liver Organogenesis — ***Daniel Guiggey***, *Ogechi Ogoke,* ***Natesh Parashurama***

Poster 164aw: Spatiotemporal Imaging and Analysis of Mouse and Human Liver Bud Morphogenesis — ***Daniel Guiggey***, *Ogechi Ogoke,* ***Natesh Parashurama***

Poster 164ax: FOXA1/2 Depletion Drives Global Reprogramming of Differentiation State and Metabolism in a Human Hepatic Cell Line and Human Stem Cell-Derived Hepatic Progenitor Cells — *Iyan Warren,* ***Daniel Guiggey***, ***Natesh Parashurama***

(165) Poster Session: Engineering Fundamentals in Life Science

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, North Hall E

Whitney Stoppel, Chair

Sponsored by: Engineering Fundamentals in Life Science

Poster 165a: Mutation of a Conserved, Hydrophobic, Cryptic Epitope Improves Manufacturability and Immunogenicity of the Sars-Cov-2 RBD — ***Sergio Rodriguez Aponte***, *Neil C. Dalvie, J. Christopher Love*

Poster 165b: Tailoring the Size of Biodegradable Poly (sulfobetaine) Hydrogels for IgG Pulmonary Delivery — ***Songpei Xie***, *Saeed Manouchehri, Joshua Ramsey, Clint Aichele*

Poster 165c: Sprayable, Antimicrobial Hydrogels to Improve Wound Infection Treatment — ***Riannon Smith***, *Nicole Brogden, Jennifer Fiegel*

Poster 165d: Constructing Zonular Articular Cartilage Using a Varied Shear Bioreactor — ***Terreill Robertson***, *Bryn Matheson, Bernard Van Wie, Arda Gozen, Ryan Driskell, Lawrence J. Bonassar, Wenji Dong, Iwona Driskell*

Poster 165e: A Comparative Assessment of the Response of Primary and Metastatic Ovarian Cancer Cells to Cisplatin in 3D Models of Various Structural and Biochemical Configurations — *Priyanka Gupta,* ***Melina Kitsiou***, *Kavitha Madhuri-Thumuluru, Aline Miller, Adedamola Olayanju, Eirini Velliou*

Poster 165g: Mouse Obesity Increases Peg-Based Micelle Liver Uptake and Decreases Lipid Nanoparticle Liver Uptake through the Modified Activity of Kupffer Cells and Lsecs — *Mitch Raith, Uche Anozie,* ***Paul Dalhaimer***

Poster 165h: Pulmonary Functionality Changes Following Titanium Dioxide Particulate Exposure and Antioxidant Protection — ***Jordan Hoops***, *Timothy Brenza*

Poster 165i: In Vitro Human Spine Model Manufacturing and Applications to Intrathecal Drug Delivery — ***Ayankola Ayansiji***, *Daniel Gehrke, Meenesh Singh, Andreas Linninger*

Poster 165j: Non-V600E Braf Mutations in Melanoma and Their Response to Different Clinically Approved Braf Inhibitors — *Erik Laurini, Maria Russi, Domenico Marson, Suzana Aulic,* ***Sabrina Pricl***

Poster 165k: Biomimetic Virus Nanoparticles for Oral Vaccine Delivery across Gut Organoid Mucosal Models — ***Qun Wang***

Poster 165l: Triggered Release of Light-Responsive Model Prodrugs from Polymeric Core-Shell Nanocarriers *Via* UV Irradiation — ***Amy Moreno***, *Jennifer Vilnot, Stefan Chassaing, Nathalie M. Pinkerton*

Poster 165m: Label-Free Optical Electrophysiology Harnessing Bio-Electrochromic Materials Interface — ***Yuecheng Peter Zhou***

Poster 165n: Characteristics of Electrically Responsive Ferrocene-Conjugated Chitosan/Alginate Hydrogel for Biomedical Application — ***Prakriti Dhungana***, *Victoria Messuri, Kyle Duke, Asma Allababdeh,* ***Byung-Wook Park***

(166) Poster Session: Food and Bioprocess Engineering

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, North Hall E

Sitanan Thitiprasert, Chair
Nuttha Thongchul, Co-Chair
Jinguang Hu, Co-Chair

Sponsored by: Food

Poster 166a: Computational Protein Analysis and Design of Aldehyde and Alcohol Dehydrogenases for Enhanced Butanol Biosynthesis in Solventogenic Fermentation — ***Curtis Moore***, *Shang-Tian Yang*

Poster 166b: Are Plant-Based Meat Alternatives More Sustainable ? — *Nicholas Schneider, Luis Huezo,* ***Rui Shi***

Poster 166c: Investigation of Antimicrobial Resistance in Listeria Monocytogenes from 2010 through 2021 — ***Robert Hanes Jr.***, *Zuyi Huang*

Poster 166d: Effect of Processing Conditions and Investigating Vitamin B-12 Retention in Fortified Soymilk Powder — ***Priya Singh***, *Kiruba Krishnaswamy, chung-Ho Lin*

Poster 166e: Enzyme Engineering of Beta-Glucosidases for Enhanced Thermal Stability and Activity — ***Emre Erkanli***, *Edward Chau, Jin Ryoun Kim*

Poster 166f: Transient Expression of Varying Gelatin Fragment Lengths in *Nicotiana Benthamiana* to Synthesize Microcarriers for Cultured Meat Production — ***Justin Wong***, *Imran Khan, Brandon Pizarro, Liber Mckee, Seongwon Jung, Patrick Negulescu, Somen Nandi, Karen A. McDonald*

Poster 166g: Enhanced Response to Non-V600E BRAF Mutations in Melanoma By Self-Assembled Nanovector Assisted Drug Delivery — *Maria Russi, Erik Laurini, Domenico Marson, Suzana Aulic,* ***Sabrina Pricl***

Poster 166i: Development of an Engineered Co-Culture Consortium for in Situ Depolymerization of Cellulose — ***Apurv Mhatre***, *Bethany Kalsheur, Thiagarajan Soundappan, Arul Mozhy Varman*

Poster 166j: Metabolic Process Engineering of *Clostridium Tyrobutyricum* Δ*cat*1::*Adh*E2 for Enhanced n-Butanol Production: Effects of Mannitol and Methyl Viologen on Flux Distribution — ***Jialei Hu***, *Jun Feng, Shang-Tian Yang*

Poster 166k: Conversion of CO_2 to Bioplastics By a Sequential Cultivation of *Clostridium Formicoaceticum* and *Pseudomonas Putida* — ***Opeyemi Bello***, *Rocky Thapaliya,* ***Forough Doustkhahvajari***, *Jie Dong*

Poster 166m: Canola Protein Production Using Different Extraction and Concentration Methods: *In Vitro* protein Digestibility, Functional Properties and Process Yields — ***Cristina Chairez Jimenez***, *Sergio Román Othón Serna-Saldívar, Cristina Chuck-Hernández*

Poster 166n: Effect of the Addition of Hydrolyzed Soybean Protein Isolate, Transglutaminase and $CaCl_2$ on the Production of Panela-Type Cheeses with Partial Substitution of Milk Protein — ***Ana Maritza Reyes-González***, *Cristina Chuck-Hernández*

Poster 499e: Engineering the Cyanobacterial Photosynthetic Electron Transport Chain to Improve Photosynthetic Efficiency — ***Nima Hajinajaf***, *Aditya Sarnaik, Parker Poole, Danika Kartchner, Amogh Deshpande, Muhammad Faisal, Kira Winsor, Jonathan Nguyen, Abhishek Singharoy, Willem Vermaas, Arul Mozhy Varman*

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(167) Poster Session: Materials Engineering & Sciences (08A - Polymers)

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, North Hall E

Caroline Szczepanski, Chair
Monirosadat Sadati, Co-Chair
Evan Wujcik, Co-Chair

Sponsored by: Polymers

ELECTROACTIVE & ELECTRONIC MATERIALS

Poster 167a: Synthesis of a Transition-Metal Based Bis-Terpyridine Functionalized Triazine Network for Electroactive Applications — ***Dana Abdullatif***, *Ahmadreza Khosropour, Alireza Abbaspourrad*

Poster 167d: MOFs-Derived Filler-Reinforced Composite Polymer Electrolyte for Solid-State Lithium-Sulfur Batteries at Room Temperature — ***Basem Al Alwan***, *Zhao Wang, K.Y. Simon Ng*

Poster 167e: Ion Conductive High Li+ Transference Number Polymer Composites for Solid-State Batteries — ***Zachary Tronstad***, *Bryan McCloskey*

MODELLING

Poster 167f: Modeling α-Olefin Copolymerization for Applications in Energy – Study of Alternatives of Synthesis — ***Funs Franco Herrero***, *Claudia Sarmoria, Adriana Brandolín, FUNS - Mariano Asteasuain*

Poster 167g: Computuationally-Efficient High-Fidellity Modelling of the High-Pressure Polymerization of Ethylene in Tubular Reactors Using Parallel Computing. — *Maira Dietrich, Claudia Sarmoria,* ***FUNS - Mariano Asteasuain***, *Adriana Brandolín*

Poster 167h: Using Drude Oscillators to Capture Ion Solvation in Generic Coarse-Grained Molecular Dynamics Simulations of Polymer Electrolytes — ***Mengdi Fan***, *Lisa Hall*

Poster 167i: Performance of Thermally Rearranged Polymers for Olefin/Paraffin Separation from All-Atom Molecular Dynamics Simulations — ***Mohammed Al Otmi***, *Janani Sampath*

Poster 167j: Effect of Dispersity on the Rheological Properties of Polyolefins from Coarse - Grained Molecular Dynamics Simulations — ***Taofeek Tejuosho***, *Janani Sampath*

Poster 167l: Computational Fluid Dynamics Analysis of Mercury Adsorption By Porous Sulfur Copolymers — ***Riffat Amna***, *Saeed Alhassan,* ***Lourdes Vega***

Poster 167m: Periodicity of Lamellar and Hexagonally Packed Cylindrical Phases in a Periodic Box — *Yuan Feng, Jiaping Wu, Baohui Li,* ***Qiang Wang***

Poster 167n: Bayesian Calibration, Validation, and Selection of Phase Field Models for Block Copolymer Self-Assembly — ***Lianghao Cao***, *J. Tinsley Oden, Omar Ghattas*

Poster 167o: Atomistic Simulation Study of a Polycarbonate/Silica Composite System: Dynamics of the Interphase — ***Lilian Johnson***, *Frederick Phelan Jr.*

Poster 167q: Polypropylene Grafted with Maleic Anhydride: A Stochastic Model. — *Tomás Romero Pietrafesa, Adriana Brandolín, Claudia Sarmoria,* ***FUNS - Mariano Asteasuain***

Poster 131d: Elucidating the Role of Network Topology Dynamics on the Coil-Stretch Transition Hysteresis in Extensional Flow of Entangled Polymer Melts — ***Mahdi Boudaghi***, *Mohammad Hadi Nafar Sefiddashti, Brian J Edwards, Bamin Khomami*

POLYMERS FOR THE ENVIRONMENT

Poster 167r: Modulation of Interfacial Tension through Amphiphilic Block Copolymer Surfactants for Environmental Sensing — ***Tyler Durkin***, *Baishali Barua, Suchol Savagatrup*

Poster 167s: Engineered Surfactants for Improved Sustainability of High Internal Phase Emulsion Polymer Foams — ***Amanda Koh***

Poster 167t: Prediction of Carbon-Dioxide Sorption in Polymer/Ionic-Liquids Systems — ***Tung Nguyen***, *Siamak Nejati, Mona Bavarian*

Poster 167u: Oxygen Tolerant Controlled Polymerization with Recyclable Micron-Scale Heterogeneous Photocatalysts — ***Kirsten Bell***, *Sarah Freeburne, Christian Pester*

Poster 167v: Consecutive Photoinduced Electron Transfers for Visible-Light Photocatalytic Polymer Synthesis — ***Alan Aguirre Soto***

Poster 167aw: Development of Hydrogel Composites for PFAS Removal in Aqueous Systems — ***Maria Victoria Klaus***, *J. Zach Hilt*

SURFACE PROPERTIES

Poster 167w: Role of the Polymer Molecular Structure and Surface Interactions on the Corrosion Resistance of Epoxy Coatings on Metals — ***Yosra Kotb***, *Christopher M. Serfass, Saad A. Khan, Lilian Hsiao, Orlin D. Velev*

Poster 167x: Reaction-Diffusion-Controlled Photopolymerization in Topographical Structures — ***Sang Deok Kim***, *Jung Gun Bae, Wonbo Lee*

POLYMERS FOR SEPARATIONS

Poster 167y: Engineering the Enhanced Li^+/Na^+ Separation Efficiency through Ionic Liquid Swollen Block Copolymer Membranes — ***Maninderjeet Singh***, *Alamgir Karim*

Poster 167z: Cs^+ Sequestration from Aqueous Media Using Hyper-Crosslinked Tetraphenylborate — ***Erwin Escobar***, *John Edward Sio, Khino Parohinog, Hern Kim, Wook-Jin Chung, Grace Nisola*

Poster 167aa: Polymers Membrane Technology for Controlled Drug Delivery System — ***Rajni Bala Talwar***

POLYMER RECYCLING & LIFE CYCLE ANALYSIS

Poster 167ac: Effect of Recycled Plastic Mixtures Blends with Coupling Agents Based Maleic Anhydride on Improving Mechanical Properties — ***Duyoung Choi***

Poster 167ad: Thermomechanical Characterization of Recyclable Diels-Alder Epoxies Loaded with TiN Nanoparticle — ***Brandon McReynolds***, *Samantha Lindholm, Kavon Mojtabai, Nicole Penners, John McCoy, Youngmin Lee, Sanchari Chowdhury*

Poster 167ae: Control of Thermomechanical Properties of a Reversible Epoxy Using Diels-Alder Chemistry — ***Gaeun Kim***, *Samantha Lindholm, Kavon Mojtabai, Brandon McReynolds, Nicole Penners, Sanchari Chowdhury, John McCoy, Youngmin Lee*

OPTICAL PROPERTIES OF POLYMERS

Poster 167af: Phase Separation-Induced Structural Color in Hydroxypropyl Cellulose Solids — ***Kyle George***, *Mohsen Esmaeili, Nader Taheri-Qazvini, Monirosadat Sadati*

SELF-ASSEMBLY

Poster 167ah: Relaxation Dynamics of Flow-Assisted Chiral Assembly — ***Mohsen Esmaeili***, *Kyle George, Nader Taheri-Qazvini, Monirosadat Sadati*

Poster 167ai: Rapid Ordering of Block Copolymer Films By Sequential Solution Immersion and Thermal Annealing with Asymmetric Reversible Processing — ***Kshitij Sharma***, *Ali Masud, Maninderjeet Singh, Sushil Satija, John F. Ankner, Jack F. Douglas, Alamgir Karim*

Poster 167aj: Nonisothermal Melt Crystallization Behavior of Semicrystalline Polymers Monitored Using an in Situ Fluorescence Technique — ***Richard Nile***, *Kailong Jin, Maya Cabello*

Poster 167ak: Synthesis and Characterization of Precision Dendritic Polymers (Dendripols) — ***Michael Dearman***, *Nduka Ogbonna, Jimmy Lawrence*

Poster 167al: Elucidating the Impact of Side Chain Dispersity in Thin Films of Bottlebrush Polymers — ***Michael Dearman***, *Nduka Ogbonna, Jimmy Lawrence*

Poster 167am: Reversible Hybridization of Sequence-Defined Oligocarbamates — ***R. Kenton Weigel***, *Christopher Alabi*

Poster 167an: Designing Hybrid Colloids: A Study of Gold Adsorption atop Polystyrene to Control Morphology of Reactive Nanoparticles — ***Joanna Schneider***, *Jason X. Liu, Victoria E. Lee, Robert K. Prud'homme, Sujit Datta, Rodney Priestley*

Poster 167ao: Hierarchical Self-Assembly of Bowtie Shaped Nanostructured Microparticles with Tunable Chiroptical Activity — ***Prashant Kumar***, *Thi Vo, Minjeong Cha, Wenqian Xu, Sharon Glotzer, Nicholas Kotov*

COMPOSITES, THERMOSETS, AND NETWORKS

Poster 167aq: High performance lignin-based coatings — ***Alessio Truncali***

Poster 167as: Prediction of Shape Recovery Performance Based Epoxy Composites Under Various Filler Types and Contents — ***Duyoung Choi***, *Sungwoong Choi*

Poster 167at: Degradation Behavior of Multilayer Packaging Films in Presence of a Highly Acidic Sauce — ***MD. Akiful Haque***, *Kerry Candlen, Amy Peterson, Jo Ann Ratto, Wan-Ting Chen*

Poster 167au: An Overview of the Fundamentals and Recent Advances in the Synthesis and Sustainable Applications of Porous Geopolymers — ***Yusuf Adewuyi***, *Monday Okoronkwo*

Poster 671h: How Adsorption Governs Chain Dynamics in Polymer Nanocomposites — ***Katelyn Randazzo***, *Rodney Priestley*

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(168) Poster Session: Materials Engineering & Sciences (08B - Biomaterials)

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, North Hall E

Evan Wujcik, Co-Chair

Sponsored by: Biomaterials

Poster 168a: Anti-biofilm Activity of Chiral Carbon Nanoparticles — ***Misché Hubbard***, *Christopher Altheim, J. Scott Van Epps, Nicholas Kotov*

Poster 168b: Biofunctional, Photodegradable Hydrogels for Discovery and Isolation of Bacteria That Drive Membrane Biofouling — ***Abigail Salberg***, *Esther Radaha, Mohammadali Masigol, Arvind Damodara Kannan, Niloufar Fattahi, Prathap Parameswaran, Ryan Hansen*

Poster 168c: Modulating the Differentiation of Human Neural Stem Cells in 3D Contexts By Varying Hyaluronic Acid Chain Length — ***Anna Gonzalez***, *Meagan McKee, Carson Koch, Andrea Jimenez-Vergara, Dany Munoz-Pinto*

Poster 168d: Graphene Quantum Dots Prevent the Amyloidogenic Tau Protein Aggregation in Alzheimer's Disease — ***Runyao Zhu***, *Youwen Zhang, Benjamin Rajewski, Kamlesh Makwana, Hyunsu Jeon, James Johnston, Juan Del Valle, Yichun Wang*

Poster 168e: Structural and Rheological Characterization of Gelation of Cranberry Oligosaccharides — ***Aniruddha Kulkarni***, *Stephen Michel, Saisumana Peddibhotla, Kirk J. Ziegler*

Poster 168f: Suture-Less Approximation of Transected Sciatic Nerve Using Biomaterial Based Nilaas — ***Mallikarjun Gosangi***, *David arturo Ruiz Pardo, Subhadeep Dutta, Shubham Pallod, Kaushal Rege*

Poster 168g: Crosslinked Alginate-Based Nanofibers for Biomedical Applications — ***Emily Diep***, *Jessica Schiffman*

Poster 168h: Silver Nanoparticles As an Effective Antimicrobial Against Otitis Media Pathogens — ***Xiaojing Ma***, *Jiayan Lang, Pengyu Chen, Rong Yang*

Poster 168i: Scalable and Modular Supramolecular and Colloidal Hydrogels for Biomedical Applications — ***Giovanni Bovone***, *Elia A. Guzzi, Stéphane Bernhard, Natthaporn Klubthawee, Mark Tibbitt*

Poster 168k: Engineering Amyloid Inspired Peptides for Tunable Assembly — ***Seren Hamsici***

Poster 168l: Delivery of Rapamycin and Basic Fibroblast Growth Factor Via Hybrid-Hydrogel for Vascular Healing — ***Luisa Palmese***, *Ming Fan, Rebecca A. Scott, Karyn G. Robinson, Huaping Tan, Robert E. Akins, Kristi L. Kiick*

Poster 168m: Shear-Induced Optical Properties in Photonic Hydroxypropyl Cellulose Solids — ***Kyle George***, *Mohsen Esmaeili, Nader Taheri-Qazvini, Monirosadat Sadati*

Poster 168n: Gelma/Gum Arabic Photocrosslinkable Microcapsules — ***James Ogilvie-Battersby***, *Daniyal Shoukat, Ramaswamy Nagarajan, Ravi Mosurkal, Nese Orbey*

Poster 168o: Biodegradable Microcapsule Designer Using Silk Fibroin Technology — ***Muchun Liu***, *Benedetto Marelli*

Poster 168p: Crosslinking Alginate-Based Nanofibers for pH-Controlled Delivery: A Study Examining Crosslinking Solution pH and Co-Solvent Systems — ***Emily Diep***, *Jessica Schiffman*

Poster 168q: Changes in Antimicrobial Efficacy Due to Ionic Binding of Modified Cellulose to Quaternary Ammonium Compounds — ***Eric Walker***

Poster 168r: *In Situ* Synchrotron to Assess the Influence of Clinical Hemodialysis Membrane Morphology on Human Serum Protein Adsorption — ***Amira Abdelrasoul***

Poster 168s: Assay and Solid-State NMR Spectroscopy of Biomembranes and Soft Materials in a Hydrogel/Particle-Based Biomimetic Material System — ***Malcolm Lane Gilchrist***, *Leo Gordon, MChem, MPhil, Robert Messinger*

Poster 168t: Multifunctional Nanodelivery System for Prostate Cancer Treatment — ***Naomi Addai Asante***, *Eviania Likos, Andrea Zuccaro, Girish Shukla, Metin Uz*

Poster 168u: Protein Resistant Polymer Coatings for Gold Nanoparticles and Surfaces — ***Christopher Ruben***, *Barrin Hendricks, Nolan Burson, Jennifer Fiegel*

Poster 168v: Engineering Lipid Nanoparticles for Controlled Spaciotemporal Release of Therapeutic Cargo to Enhance Cell Survivability during Stem Cell Transplant Therapy — ***Rashi Porwal***, *Li Han, Stephen L. Hayward, Yuguo Lei, Srivatsan Kidambi*

Poster 168w: *Translating Polymeric Vehicles between Ribonucleoprotein and Plasmid DNA Cargoes: Do the Same Design Rules Apply?* — ***Ramya Kumar***, *Ngoc Le, Mary Brown, Theresa M. Reineke*

Poster 168x: Chirality-Assisted Drug Delivery in Exosomes for Gene Therapy — ***Youwen Zhang***, *Yichun Wang, Hsueh-Chia Chang, Ceming Wang, Runyao Zhu, Hyunsu Jeon, James Johnston*

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(169) Poster Session: Materials Engineering & Sciences (08D - Inorganic Materials)

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, North Hall E

Xueyi Zhang, Chair
Evan Wujcik, Co-Chair

Sponsored by: Inorganic Materials

Poster 169a: Engineering Seed-Assisted Syntheses of Pentasil Zeolite Nanosheets — ***Muhammad Fiji***, *Rishabh Jain, Jeffrey Rimer*

Poster 169b: Elucidating the Mechanism of Faujasite Crystallization By in Situ Scanning Probe Microscopy — ***Zhiyin Niu***, *Rishabh Jain, Madhuresh Choudhary, Jeffrey Rimer*

Poster 169c: Crystallization of NiO Exposing High-Index Facets By Molten Salt Synthesis — ***Mariano D. Susman***, *Hien N. Pham, Xiaohui Zhao, Raffaele Cheula, David West, Sivadinarayana Chinta, Matteo Maestri, Praveen Bollini, Abhaya K. Datye, Jeffrey Rimer*

Poster 169d: Choreographing Zeolite Crystallization: It's Elementary — ***Adam J. Mallette***, *Sungil Hong, Giannis Mpourmpakis, Jeffrey Rimer*

Poster 169e: Bond-Valence Parameterization for the Accurate Description of DFT Energetics in ABO_3 Perovskite Oxides — ***Ryan Morelock***, *Zachary Bare, Charles B. Musgrave*

Poster 169f: Beyond Interfacial Resistance: Interface Design for Dendrite-Free All-Solid-State Lithium Metal Batteries (same as student awards submission) — ***Xinzi He***, *Chunsheng Wang*

Poster 169g: Synthesis and Characterization of Substituted Aluminophosphates for Oxygen-Nitrogen Separation — ***Natalia Ali***, *Steven Wilson, Ellen B. Stechel, Ivan Ermanoski, Christopher Muhich, Shuguang Deng*

Poster 169h: Studying the Synthesis of Hierarchical Siliceous Zeolites By Post Synthetic Zeolite Surfactant-Templating Method — ***Kaivalya Gawande***, *Wei Fan*

Poster 169i: Utilizing Magnetic Heating of Coni Nanoparticles for Electrifying Chemical Conversions — ***Anja Sedminek***, *Darko Makovec, Petra Jenus, Janvit Terzan, Blaž Likozar, Sašo Gyergyek*

Poster 169j: Magnesium Oxychloride Composites: Design, Synthesis and Scaled-up Manufacturing for Next Generation Building Materials — ***Christopher Kitchens***

Poster 169k: Influence of Reaction Parameters on the Exsolution of Ni-Ru Bimetallic Alloy in GEO-Inspired Perovskite — ***Somchate Wasantwisut***, *Kandis Leslie Abdul-Aziz*

Poster 562g: Structure-Property Relation of Ti_3C_2 Mxene/Polyelectrolyte Hybrid Films — ***Farivash Gholamirad***, *Nader Taheri-Qazvini*

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(170) Poster Session: Materials Engineering & Sciences (08E - Electronic and Photonic Materials)

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, North Hall E

Elizabeth Lee, Chair
Evan Wujcik, Co-Chair

Sponsored by: Electronics and Photonics

Poster 170a: SMART Solar Transmittance Modulation in Newly Engineered Organic Molecules with Multistimulated Optical Switchability and Reversibility — ***John Marc C. Puguan***, *Pramod V. Rathod, Grace Nisola, Wook-Jin Chung, Hern Kim*

Poster 170b: Acute Exposure to e-Cigarette Vapor Promotes Neutrophil-Platelet Aggregation in Murine Pulmonary Microvasculature — *Hunter Snoderly,* ***Hassan Alkhadrawi***, *Dhruvi Panchal, Margaret Bennewitz*

Poster 170c: Engineering a Colloidal Metamaterial Comprising of Metamaterial-Capped Janus Particles for Light Harvesting Applications in Cancer Detection and Therapeutics — ***Samhita Kattekola***, *Ilona Kretzschmar, Alexander Couzis*

Poster 170e: State of Charge Estimation of Lithium-Ion Battery Using Surrogate Model Based on Electrochemical-Thermal Model — ***Seunghyeon Oh***, *Jiyong Kim, Il Moon*

Poster 170f: Ionic Liquid-Reinforced Carbon Nanofiber Matrix Enabled Lean-Electrolyte Li-S Batteries Via Electrostatic Attraction — ***Xinyang Wang***, *Yingying Lu*

Poster 170g: Impact of Dispersion Processing on Ionomer Thin Films — ***Ashley Bird***, *Ahmet Kusoglu*

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(171) Poster Session: Materials Engineering & Sciences (08F - Composite Materials)

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, North Hall E

Evan Wujcik, Co-Chair

Sponsored by: Composites

Poster 171a: Patch Repair of Composites Using Dielectric Barrier Discharge Induced Heating and Curing — ***Anubhav Sarmah***, *Smita S. Dasari, Micah Green*

Poster 171b: Mechanically Robust Egyptian Blue Coated “Super Marbles” — ***Agoston Kiss***, *Holly A. Stretz*

Poster 171c: Thermal Stability and Flammability Studies of Mxene–Organic Hybrid Polystyrene Nanocomposites — ***Zhuoran Zhang***, *Huaixuan Cao, Emily Pentzer, Micah Green, Qingsheng Wang*

Poster 171e: Parametric Study of Type-IV Hydrogen Pressure Vessel to Predict the Buckling of Polymeric Liner Under Thermo-Mechanical Load — ***Akash Burolia***, *Jigyasa Daiya, Pranjali Sharma, Swati Neogi*

Poster 171f: Bioinspired, Conductive Polymeric Composites of End-Capped Oligopeptides — ***Prerana Rathore***, *Brian Montz, Stephen Nonnenmann, Todd Emrick, Jessica Schiffman*

Poster 171g: Magnetic Graphene Oxide Grafted with Temperature-Responsive Crown Ether Polymer Brushes As an Adsorbent for Lithium Recovery from Seawater — ***Khino Parohinog***, *Negasi Teklay Weldesemat, John Edward Sio, Grace Nisola, Wook-Jin Chung*

Poster 171h: 3D Printing of Poly-Dimethyl Siloxane (PDMS)/Liquid Metal Composites for Micro-Patterning Applications — ***Dhanush Patil***

Poster 171i: Sustainable Recycling of Crosslinked Polyethylene (XLPE) Via Foam Engineering — ***Mohammed Bawareth***, *Kenan Song*

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(172) Poster Session: Pharmaceutical Discovery Development and Manufacturing (PD2M)

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, North Hall E

Andreas Bommarius, Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

Poster 172a: AI-Driven Drug Discovery and Manufacturing Using Automated Ontology-Based Information Extraction — ***Vipul Mann***, *Shekhar Viswanath, Shankar Vaidyaraman, Jeyakumar Balakrishnan, Jon Dieringer, Venkat Venkatasubramanian*

Poster 172b: Deciphering Longitudinal Optical-Density Measurements to Guide Antibiotic Use: A Model Based Approach — ***Iordanis Kesisoglou***, *Vincent H. Tam, Michael Nikolaou*

Poster 172c: A Mathematical Model to Predict the Drug Release Profile in Bilayered Osmotic Controlled Release Tablets — ***Bhawana Tomar***, *Mahesh S. Tirumkudulu, Sweta Manthena, Weili Yu, Alfred Berchielli, Pankaj Doshi*

Poster 172d: Preparation of Stable Nanoparticles of Curcumin in a Single Step — ***Parimaladevi Palanisamy***, *Vasanth Kumar Kannuchamy, Sean Costello, Gavin Walker*

Poster 172e: The Batten disease gene product CLN3 is required for the clearance of glycerophosphodiesters from lysosomes — *Nouf Laqtom,* ***Wentao Dong***, *Uche Medoh, Andrew Cangelosi, Vimisha Dharamdasani, Sze Ham Chan, Tenzin Kunchok, Caroline A. Lewis, Ivonne Heinze, Rachel Tang, Christian Grimm, An Dang Do, Forbes Porter, Alessandro Ori, David Sabatini, Monther Abu-Remaileh*

Poster 172f: Untargeted metabolomic and lipidomic profiling for Golgi molecular content via immunoprecipitation (Golgi-IP) — ***Wentao Dong***, *Rotimi Fasimoye, Raja Nirujogi, Eshaan Rawat, Miharu Iguchi, Uche Medoh, Kwamina Nyame, Dario Alessi, Monther Abu-Remaileh*

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(173) General Poster Session

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, North Hall E

Sponsored by: Poster Sessions

Poster 173b: Waste Plastic Upcycling: Microkinetic Modelling of Hdpe Pyrolysis — ***Aswathy Raghu***, *Rebecca Harmon, SriBala Gorugantu, Linda Broadbelt*

Poster 173d: Multiscale Modeling Approach for Designing Novel Hierarchical Carbon Cathodes for Ultrahigh Capacity Aprotic Li-O_2 Battery — ***Khizar Hayat***, ***Daniel Bahamon***, *Lourdes Vega, Ahmed Al Hajaj*

Poster 173f: Demonstrating the Affect of Polymer Type on Oil Yield in Thermal Depolymerization Using Machine Learning — ***Elizabeth Belden***, *Owen Ferrara, Matthew Rando, Eric Himebaugh, Christopher Skangos, Randy Paffenroth, Nikolaos Kazantzis, Michael T. Timko*

Poster 173h: Tuning C-Phycocyanin Photoactivity Via pH-Mediated Assembly–Disassembly — *Ying Li,* ***Alireza Abbaspourrad***, *Richard Gillilan*

Poster 173i: Study on Growth and Metabolite Trend Comparison of *Staphylococcus Aureus* and *Pseudomonas Aeruginosa* in Monoculture and Co-Culture System — ***Heejoon Park***

Poster 173j: A Deep Learning-Based Feature Extraction Framework for Monitoring High-Order Nonstationary Industrial Processes — ***Cheng Ji***, *Tingting Tao, Fangyuan Ma, Jingde Wang, Wei Sun*

Poster 173k: Machine Learning Analysis of Multimodal Data from a Smartphone-Based Electrochemiluminescence Sensor. — ***Hyun Kwon***, *Elmer Ccopa Rivera, Rodney Summerscales*

Poster 173o: *Production of Novel Sars-Cov-2 Spike Truncations in Chinese Hamster Ovary Cells Leads to High Expression and Binding to Antibodies* — ***Shiaki Minami***, *Seongwon Jung, Yihan Huang, Bradley Harris, Matthew Kenaston, Roland Faller, Somen Nandi, Karen A. McDonald, Priya Shah*

Poster 173p: Microed: Cryo-Electron Diffraction of 3D Microcrystals — ***Alison Haymaker***, *Brent L. Nanenga*

Poster 173q: Understanding Protein Mediated Biomineralization Using Cryogenic Electron Microscopy — ***Sagnik Sen***

Poster 173s: Photoelectrochemical Reduction of Oxygen on Two-Dimensional Covalent Organic Frameworks — ***Syed Ibrahim Gnani Peer Mohamed***, *Amir Shariffar, Christopher Merkel, Mona Bavarian, Siamak Nejati*

Poster 173ah: Discovering Latent Effective Parameters from Heterogeneous Populations — ***Nikolaos Evangelou***, *George Kevrekidis, Felix Dietrich, Ioannis G. Kevrekidis*

Poster 173ai: Insight to Crystallisation Fouling from 4D X-Ray: A Three Step Process? — *Isaac Appelquist, Peter Winkel Rasmussen, Henning Osholm, Anders Nymark Christensen, Anders Bjorholm Dahl, Philip Loldrup Fosbøl,* ***Benaiah Anabaraonye***

Poster 173aj: Inter-Electronic and Inter-Valley Transitions in MoS_2-WS_2 Heterostructures and Alloys — ***Sungjoon Kim***, *Vikas Berry*

Poster 173ak: Bacterial Conversion of Methane to Lipids: A Technical Assessment and Benefit-to-Cost Analysis As Methane Abatement Strategy — ***Lisa Stephanie Dizon***, *Robert Bertrand, William Holmes, Rafael Hernandez, Mark Zappi, Dhan Lord Fortela, Emmanuel Revellame*

Poster 173al: Computational Design of Therapeutic Drug Formulations to Control Protein Interactions — ***Gregory Dignon***

Poster 173am: A Novel Application of the Newcomb-Benford Law to Exposure Data — ***Byron Fuentes***, *Öyku Dinçkol, Spyros Karakitsios, Dimosthenis Sarigiannis, Silvia Valentini, Elena De Felip, Laura Ricceri, Gemma Calamandrei, Anna Pino, Dayna Schultz*

Poster 173an: Deepcdp: Deep Learning Charge Density Prediction — ***Siddarth Achar***, *Leonardo Bernasconi, Karl Johnson*

Poster 173ao: The Saturation Dependence of $BaSO_4$ Surface Precipitation Kinetics — *Isaac Appelquist,* ***Benaiah Anabaraonye***, *Philip Loldrup Fosbøl*

Poster 173ap: High-Temperature Corrosion in Waste-to-Energy (WtE) Boilers and Cement Kiln — ***Janhvi Trivedi***, *Marco J. Castaldi*

Poster 173aq: A KMC Based Tool to Understand the Chemical Recycling of Polyurethanes — ***SriBala Gorugantu***, *Matthew W. Coile, Obonetse Kebadireng, Linda Broadbelt*

Poster 173ar: Characterisation of the Crystal Polymorphs of Polyvinylidene Fluoride Using FTIR, Raman and DSC Measurements — ***Shubham Mireja***, *Devang Khakhar*

Poster 173as: Hollow Fiber Membranes for Evaporative Cooling — ***Andrew Lin***, *Dibakar Bhattacharyya*

Poster 173at: Integrated production of chemicals and fuels in the pulpindustry: techno-economic and environmental analysis ofblack liquor gasification-based processes — *Meire Ellen Gorete Ribeiro Domingos, Daniel Florez-Orrego, Silvio de Oliveira Junior, François Maréchal,* ***Moises Santos***

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(174) Panel: Supporting and Investing in early stage startups

Monday, Nov 14, 10:45 AM
Phoenix Convention Center, W-103B

Henry Uyeme, Chair
Daniel Kriozere, Co-Chair

Sponsored by: Entrepreneurship in Chemical Engineering

10:45 Paper 174a: Innovation Fellowship: Novel Postdoctoral Training to Build a Pipeline of Innovation-Minded Professionals and Promote Commercialization in Academic Units — ***Anastasiia Visheratina****, Dylan Neale, Kaylee Steen, Elizabeth Herness Peters, Nadine Wong, Joerg Lahann*

11:10: Panel Discussion: Stephen Sims, Laura Silva, Robert Sovesky, Vera Schroeder, and Jonathan Girroir

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(175) 25th Anniversary of The Catalysis and Reaction Engineering Division III (Invited Talks)

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-129AB

Bihter Padak, Chair
Omar Abdelrahman, Co-Chair
Randall Meyer, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

3:30 Paper 175a: The Engineering of Catalytic Condensers for Programmable Chemistry — ***Paul Dauenhauer***

3:55 Paper 175b: Data-Centric Chemical Reaction Engineering for Energy Transition — ***Ryan Hartman***

4:20 Paper 175c: Thermodynamics of Environment-Dependent Chemisorption on Metal Surfaces Versus Metal Oxo Cations — *Stephen Vicchio, Jiazhou Zhu, Sean T. Dix, Hafeera Shabbir,* ***Rachel Getman***

4:45 Paper 175d: Electronic, Ensemble, and Coverage Effects in PdCu Alloys: From Segregated Bulk Systems to Dilute Surface Alloys Down to the Single Atom Limit — ***Lars Grabow***

5:10 Paper 175e: Embracing the Complexity of Catalytic Structures: Engineering Nonstoichiometric Mixed Metal Oxides for Electrocatalysis — ***Eranda Nikolla***

5:35 Paper 175f: A Light in the Dark: Leveraging High-Throughput Simulations to Navigate the Complex Energetic Landscape of Templating Organic Molecules Used for Zeolite Synthesis — *Daniel Schwalbe-Koda, Soonhyoung Kwon, Cecilia Paris, Estefania Bello-Jurado, Zach Jensen, Elsa Olivetti, Tom Willhammar, Avelino Corma,* ***Yuriy Roman****, Manuel Moliner, Rafael Gomez-Bombarelli*

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(176) Catalysis in Liquid Media II: Impact of Liquid Phase on Adsorption and Conversion in Catalysis

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-127B

Jean-Sabin McEwen, Chair
Deven Swapneshu Baser, Co-Chair

Sponsored by: Catalysis

3:30 Paper 176a: Dynamically Formed Active Sites on Liquid Boron Oxide for Selective Oxidative Dehydrogenation of Propane — *Jinshu Tian,* ***Gregory Collinge****, Simuck Yuk, Jingdong Lin, Wei Shou, Vassiliki-Alexandra Glezakou, Mal-Soon Lee, Yong Wang, Roger Rousseau*

3:48 Paper 176b: Interfacial Sites Determine Paths of O_2 and H_2 Activation on Au Nanoparticles: Effects of Nanoparticle Size and Support Identity on O_2 Reduction in Aqueous Media — ***Jason Adams****, Tomas Ricciardulli, Abinaya Sampath, David Flaherty*

4:06 Paper 176c: Liquid Phase Effects on Adsorption Processes over Metal Surfaces — ***Dia Sahsah****, Andreas Heyden*

4:24 Paper 176d: The Role of Water in Aldol Condensation of Cyclopentanone on Functionalized-MgO Surface: A DFT Mechanistic Study — ***Yu Yan****, Bin Wang*

4:42 Paper 176e: Influence of Olefin-Surface Interactions on Liquid-Phase Activity of Silica-Supported Mo-Based Olefin Metathesis Catalysts — ***Zachariah Berkson****, Gregory Price, Glenn Sunley, Christophe Copéret*

5:00 Paper 176f: Effect of Water Concentration on Rates and Selectivities of Alkene Epoxidations in Ti-BEA Zeolites — ***David Potts****, Ohsung Kwon, David Flaherty*

5:22 Paper 176g: Kinetic Modeling of Electrocatalysis in Electrolytic Media Using Dimensional Analysis: Bridging Electrocatalytic Systems of Different Mass Transport Characteristics — ***Joonbaek Jang****, Carlos Morales-Guio*

5:40 Paper 176h: The Role of Competitive Water Adsorption in Controlling Anodic Dinitrogen Activation — ***Joseph Gauthier***

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(177) Catalyst Design, Synthesis, and Characterization III: Structure/activity relationships

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-127C

Madelyn Ball, Chair
Michael Nigra, Co-Chair

Sponsored by: Catalysis

3:30 Paper 177a: Highly Active and Stable $Pt_1/CeO_x/SiO_2$ Single-Atom Catalyst for CO Oxidation — ***Yiwei Yu****, Jingyue Liu*

3:48 Paper 177b: Understanding Surface Structures and Reactivity of Heterogeneous Olefin Metathesis Catalysts through Sensitivity-Enhanced Solid-State NMR — ***Zachariah Berkson****, Terry Z. H. Gani, Ran Zhu, Yuriy Roman, Christophe Copéret*

4:06 Paper 177c: Exploring Pt-Wox Interactions in Hydrodeoxygenation Catalysts for Lignin Upgrading — ***Justin Marlowe****, Mahdi Abu-Omar, Phillip Christopher*

4:24 Paper 177d: Elucidating the Roles of Nanoparticle Clustering and Equilibrium Heating in Plasmonic Catalysts Under Continuous Broadband Illumination — ***Rachel Elias****, Suljo Linic*

4:42 Paper 177e: Metal-Metal Oxide Interaction Induced Yolk-Shell Nanocrystals for Acetylene Semihydrogenation — ***Zihao Yan****, Huiyuan Zhu*

5:00 Paper 177f: Synthesis of Well-Defined IrO_2/TiO_2 Catalysts for Low-Temperature Activation of Methane — ***Helena Hagelin Weaver****, Bochuan Song, Li-Yin Hsiao*

5:18 Paper 177g: Towards Enhancing the Reactivity in Olefin Metathesis over Bimetallic Monb Single Site Catalyst — ***Anoop Uchagawkar****, Denis Johnson, Anand Ramanathan, Bala Subramaniam*

5:36 Paper 177h: Higher Density of Supported Single-Atom Pt_1 Metal in the Pt/α-Moc Catalysts Renders Lower Intrinsic Activity for the Reverse Water Shift Reaction — ***Ewa Chukwu****, Lindsay Molina, Conner Rapp, Luis Morales, Hui Wang, Sungsik Lee, Stavros Karakalos, Ming Yang*

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(178) Environmental Catalysis III: Emerging Catalytic Technologies

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-227B

Fudong Liu, Chair
Max Huelsey, Co-Chair
Santhosh Gundlapally, Co-Chair
Harsha Surenahalli, Co-Chair

Sponsored by: Catalysis

3:30 Paper 178a: Patterned Cu-Ti Bimetallic Oxides for Electrooxidation of Methane to Methanol at Ambient Conditions — ***Rohan Sartape****, Aditya Prajapati, Nishithan Balaji Chidambara Kani, Meenesh Singh*

3:50 Paper 178b: Detailed Mechanistic Studies of Catalysts on Real Feeds for Ultra-Low-Sulfur Diesel Production — ***Yi Du***, *Michael R. Harper, Bradley Wooler*

4:10 Paper 178c: Theoretical Insights into the Photocatalytic PFOA Degradation Mechanism over Boron Nitride — ***Yu Chen***, *Manav Bhati, Thomas Senftle*

4:30 Paper 178d: Reactive Stability of Polymorphic Iron-Based Metal-Organic Frameworks in Green Oxidant Driven Aqueous Pollutant Degradation — ***Samuel Moore***, *Michele Sarazen*

4:50 Paper 178e: Aqueous Phase Hydrodechlorination of Trichloroethylene Using Pd Supported on Swellable Organically Modified Silica (SOMS): Effect of Support Derivatization — ***Anagha Hunoor***, *Saurabh Ailawar, Dishari Basu, Benjamin Rudzinski, Laurence Burel, Jean-Marc Millet, Jeffrey Miller, Paul Edmiston, Umit Ozkan*

5:10 Paper 178f: Catalytic Methane Steam Reforming with Ni-xMo2C/FAU: Formation Energetics and Promoting Role of Molybdenum Carbide Clusters Encapsulated — *Xianghui Zhang, Margaret Reece, Andrew Strzelecki, Cody B. Cockreham, Vitaliy Goncharov, Houqian Li, Kyungmin Yim, Jinsoo Kim, Junming Sun, Hui Sun, Baodong Wang, Xiaofeng Guo, Hongwu Xu, Su Ha, Yong Wang,* ***Di Wu***

5:30 Paper 178g: Understanding the Role of Branching on Thermal and Catalytic Polyethylene Decomposition Reactions — ***Ana Carolina Roncoli Jerdy***, *Pascale Attalah, David Soules, Ron Abbott, Lobban Lance, Steven Crossley*

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(179) Fundamentals of Catalysis and Surface Science III: Kinetics of surface reactions

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-128B

Manish Shetty, Chair
Nathaniel Eagan, Co-Chair

Sponsored by: Catalysis

3:30 Paper 179a: Trends of Heteroatom and Metal Identities in C–X Hydrogenolysis — ***Nikki Kragt***, *Abdulrahman Almithn, David Hibbitts*

3:50 Paper 179b: Rates and Reversibilities in Interconnected Reaction Networks — ***Ting Lin***, *Neil Razdan, Aditya Bhan*

4:10 Paper 179c: A Parameterization Strategy for Coverage-Dependent DFT-Based Microkinetic Modeling of Surface Catalytic Reactions — ***Anshuman Goswami***, *William Schneider*

4:30 Paper 179d: Rate Expressions in Mean Field Microkinetic Models Incorporating Multiple Types of Active Sites — ***Gregory Collinge***, *Devyani Sharma, Jean-Sabin McEwen, Mark Saeys*

4:50 Paper 179e: Rate Analysis of a Curious Case of (Side) Product Inhibition — *Xiaohui Zhao, Jeffrey Rimer,* ***Praveen Bollini***

5:10 Paper 179f: Measurements of Structure Sensitivity Spanning Surface Orientation Space — ***Andrew Gellman***, *Carlos Fernandez-Caban*

5:30 Paper 179g: Predicting Activation Energies of Transition Metal Nanoparticle Reconstruction Via an Interaction-Counting Approach — ***Deep M. Patel***, *Luke Roling*

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(180) Reaction Path Analysis

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-128A

Manjiri Moharir, Chair
Peter Valdez, Co-Chair

Sponsored by: Reaction Engineering

3:30 Paper 180a: Mechanistic Investigations into the Hydrolysis of Carbonyl Sulfide on Metal Oxides By Ab-Initio Simulations — ***Pranav Kherdekar***, *Shantanu Roy, Divesh Bhatia*

3:55 Paper 180b: Understanding the Complex Reaction Network of Model Polyolefin Upcycling Via Informatics and Machine Learning — ***Chin-Fei Chang***, *Srinivas Rangarajan*

4:20 Paper 180c: Revealing Molecular-Level Interactions and Kinetics of Cellulose Decomposition during Its Co-Pyrolysis with Lignin — ***Fuat Sakirler***, *Hsi-Wu Wong*

4:45 Paper 180d: Accelerating the Process of Combustion Mechanism Discovery through Correlated Uncertainty and Sensitivity Analysis — ***Sevy Harris***, *Carly LaGrotta, Mark Barbet, Michael Burke, Richard West*

5:10 Paper 180e: Metal-Organic Framework Catalysts for Chemical Upgrading Reactions — ***Saumil Chheda***, *Dong Yang, Katherine McCullough, Daniel King, Joern Siepmann, Massimiliano Delferro, Bruce C. Gates, Laura Gagliardi*

5:35 Paper 180f: Mechanistic Insights into the Cobalt-Catalyzed Fischer-Tropsch Synthesis — ***G. T. Kasun Kalhara Gunasooriya***

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(181) Recent Advances in Molecular Modeling of Interfacial Thermodynamics and Dynamics

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-222B

Gul Zerze, Chair
Michael Howard, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

3:30 Paper 181a: Optiboost: A Method for Choosing a Safe and Efficient Boost for the Bond-Boost Method in Accelerated Molecular Dynamics Simulations with Hyperdynamics — ***Jianming Cui***, *Kristen Fichthorn*

3:45 Paper 181b: Coupling Replica Exchange with Backbone sampling Captures Conformational Changes on Protein-Protein Interfaces — ***Ameya Harmalkar***, *Jeffrey J. Gray*

4:00 Paper 181c: Molecular Modes from NMR Relaxation in Fluids: Going Beyond the Bpp Theory — ***Arjun Valiya Parambathu***, *Philip Singer, Thiago Jose Pinheiro Dos Santos, George J. Hirasaki, Walter Chapman, Dilip Asthagiri*

4:15 Paper 181d: Unbiased Coarse-Grained Monte Carlo Simulation Using SAXS-Data for Identification of Self-Assembled Nanostructures — ***Silabrata Pahari***, *Shuhao Liu, Mustafa Akbulut, Joseph Kwon*

4:31 Paper 181e: Equilibrium Adsorption Morphologies of Surfactants at Metal-Water Interfaces Studied Using a Novel Free Energy Sampling Methodology in Molecular Simulations — ***Sumit Sharma***, *Himanshu Singh*

4:46 Paper 181f: A Molecular Dynamics Simulation Study of the Kapitza Heat Transfer Resistance — ***Sebastian Schmitt***, *Simon Stephan, Hans Hasse*

5:01 Paper 181g: Molecular Modeling of Alcohol Effects in Nonionic Surfactant Micelles with Density Functional Theory — ***Jinxin Lu***, *Walter Chapman*

5:16 Paper 181h: Extracting Solid-Melt Interfacial Free Energy and Anisotropy Strength of Al-Cu Alloy Using Molecular Dynamics Simulations — ***Amrutdyuti Swamy***, *Pabitra Choudhury, Daniel Dolce*

5:31 Paper 181i: Molecular Dynamics Simulation of O2 Transport in Nafion — ***Nicholas Tiwari***

5:46 Paper 181j: Coarse-Grained Molecular Dynamics Investigation of Adsorption of Type IV Pili Proteins Onto Graphene-Cu(111) and Defective Graphene-Cu(111) Interfaces — ***Sourav Verma***, *Marina Davidson, Kenneth Benjamin*

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(182) Data-Driven Dynamic Modeling, Estimation and Control III

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, W-101B

Joel Paulson, Chair
Utkarsh Shah, Co-Chair

Sponsored by: Systems and Process Control

3:30 Paper 182a: Data-Driven Discovery of Sparse Dynamical Model of Cardiac System for Model Predictive Control — ***Siddharth Prabhu***, *Srinivas Rangarajan, Mayuresh Kothare*

3:49 Paper 182b: Convex Optimal Control of Multi-Time-Scale Systems Using Input Convex Temporal Convolutional Neural Networks — ***Shu Yang***, *Sambit Ghosh, Ungorr Nassery, B Wayne Bequette*

4:08 Paper 182c: Predicting Goal Attainment in Control-Oriented Behavioral Interventions Using a Data-Driven System Identification Approach — ***Sarasij Banerjee***, *Rachael Kha, Daniel Rivera, Eric Hekler*

4:27 Paper 182d: Modeling Tipping Points in the Reduced-Order Stochastic Dynamics of a Population of Interacting Agents — ***Cristina Martin Linares***, *Tianqi Cui, Gianluca Fabiani, Nikolas Evangelou, Constantinos Siettos, Ioannis G. Kevrekidis*

4:46 Paper 182e: Reduced-Order Modeling and Predictive Control of Nonlinear Processes Using Machine Learning — *Tianyi Zhao, Yingzhe Zheng,* ***Zhe Wu***

5:05 Paper 182f: Recovery of Transparent Dynamic Models from Black-Box Systems Using Symbolic Regression. — ***Benjamin Cohen***, *Burcu Beykal, George M. Bollas*

5:24 Paper 182g: Process Aware Data Driven Modeling and Model Predictive Control of Monoclonal Antibody Bioreactor — *Samardeepsingh Sarna,* ***Nikesh Patel***, *Brandon Corbett, Chris McCready, Prashant Mhaskar*

5:43 Paper 182h: Learning Linear Representations of Nonlinear Dynamics Using Deep Learning — ***Akhil Ahmed***, *Antonio del Rio Chanona, Mehmet Mercangoez*

(183) Advances in Process Design

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, W-101A

Alexander Dowling, Chair
Shachit Iyer, Co-Chair

Sponsored by: Systems and Process Design

3:30 Paper 183a: Synthesis of Coffee Wastewater Treatment Network with Single Input and Multiple Output Streams Using the P-Graph Framework — ***Emmanuel Aboagye***, *Quint Kearns, Jean Pimentel, Akos Orosz, Heriberto Cabezas, Ferenc Friedler, Kirti Yenkie*

3:45 Paper 183b: Superstructure Synthesis and Simulation-Optimization of Pharmaceutical Manufacturing Processes Using Pharmapy — ***Daniel Laky***, *Daniel Casas Orozco, Gintaras Reklaitis, Zoltan Nagy*

4:00 Paper 183c: Simultaneous Process Design & Optimisation: An Application to Bioprocesses — ***Steven Sachio***, *Cleo Kontoravdi, Maria M. Papathanasiou*

4:15 Paper 183d: Flowsheet Synthesis through Graph-Based Reinforcement Learning — *Roel J. Leenhouts, Laura Stops, Shachi M. Shanbhag, Qinghe Gao,* ***Artur M. Schweidtmann***

4:30 Paper 183e: Process Synthesis for the Valorisation of Low-Grade Heat: Geothermal Brines and Industrial Waste Streams — *Victor M. García-Anteportalatina,* ***Mariano Martin***

4:45 Paper 183f: Mathematical Modeling and Economic Optimization of a Novel Amine-Based Post-Combustion Carbon Capture Process — ***Ilayda Akkor***, *Shachit S. Iyer, John Dowdle, Le Wang, Chrysanthos Gounaris*

5:00 Paper 183g: Integrated Membrane Material Design and System Synthesis — ***Garry S.P. Taifan***, *Christos Maravelias*

5:15 Paper 183h: Mathematical Programming Formulations for Design and Manufacturing of Process Families: Applications to Green Energy Systems — ***Georgia Stinchfield***, *Michael Bynum, Miguel A. Zamarripa, John Siirola, Carl Laird*

(184) Area Plenary: Future Directions in Applied Mathematics and Numerical Analysis (Invited Talks)

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, W-102A

Satyajith Amaran, Chair
Kamil Khan, Co-Chair

Sponsored by: Applied Mathematics and Numerical Analysis

3:30 Paper 184a: Model-Based Control of Epithelial-Mesenchymal Transition through Signaling Regulation in Pancreas Cancer Cells — ***Varghese Kurian***, *Michelle Barbeau, Yu Luo, Janine Buonato, Babatunde A. Ogunnaike, Matthew Lazzara*

3:55 Paper 184b: Machine Learning and Mechanism-Based Mathematical Modeling to Identify Biomarkers and Mechanisms behind Severe Pediatric Influenza Infection — ***Lauren Luciani***, *Brydie R. Huckestein, John Alcorn, Jason E. Shoemaker*

4:20 Paper 184c: Quantum Algorithms for Calculating Light-Absorption and Thermal Properties of Molecules and Materials — ***Nicolas P. D. Sawaya***

4:45 Paper 184d: Development of a Deterministic Optimization Approach, the Sdnbi Algorithm for Nonconvex and Combinatorial Bi-Objective Programming and Its Application to Molecular Design — ***Ye Seol Lee***, *Amparo Galindo, George Jackson, Claire Adjiman*

5:10 Paper 184e: A Feasible Path-Based Branch and Bound Algorithm for Strongly Nonconvex MINLP Problems in Process Synthesis and Intensification — ***Chao Liu***, *Yingjie Ma, Jie Li*

5:35 Paper 184f: Modeling of Multi-Dimensional Dynamics Using Layered Algorithms: Application to Lignin Depolymerization and Self-Assembly Simulation with Experimental Validation — ***Juhyeon Kim***, *Silabrata Pahari, Joseph Kwon*

(185) Data Science/Analytics for Process Applications

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, W-101C

Matthew Ellis, Chair
Xunyuan Yin, Co-Chair

Sponsored by: Information Management and Intelligent Systems

3:30 Paper 185a: Data Fusion and Feature Selection for Process Monitoring at Hanford — ***Steven Crouse***, *Rupanjali Prasad, Stefani Kocevska, Ronald Rousseau, Martha Grover*

3:49 Paper 185b: A Comprehensive Causation Prediction Model of Pipeline Incidents Using Artificial Neural Network — ***Pallavi Kumari***, *Qingsheng Wang, Faisal Khan, Joseph Kwon*

4:08 Paper 185c: Data-Driven Feasibility and Performance Prediction of Production Scheduling MIP Models — ***Boeun Kim***, *Christos T. Maravelias*

4:27 Paper 185d: Machine Learning-Based Operational Modeling of an Electrochemical Reactor: Handling Data Variability and Improving Empirical Models — ***Junwei Luo***, *Vito Canuso, Joonbaek Jang, Zhe Wu, Carlos Morales-Guio, Panagiotis Christofides*

4:46 Paper 185e: A Graph-Based Software Framework for Data Science — ***David Cole***, *Victor Zavala*

5:05 Paper 185f: Machine Learning-Based Ethylene Concentration Estimation, Real-Time Optimization and Feedback Control of an Experimental Electrochemical Reactor — ***Berkay Citmaci***, *Junwei Luo, Joonbaek Jang, Vito Canuso, Derek Richard, Yi Ming Ren, Carlos Morales-Guio, Panagiotis Christofides*

5:24 Paper 185g: Optimization Methods for Exploring Accuracy Versus Robustness of a Regression Prediction in Process Analytical Technology — ***Chrysoula Kappatou***, *James Odgers, Salvador Garcia Munoz, Ruth Misener*

5:43 Paper 185h: Data-Driven Techniques Towards the Efficient Integration of Planning, Scheduling and Control — ***Damien van de Berg***, *Nilay Shah, Antonio del Rio Chanona*

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(186) Modernization and Integration of the ChE Curriculum

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, W-105B

Katie Cadwell, Chair
Taryn Bayles, Co-Chair

Sponsored by: Undergraduate Education

3:30 Paper 186a: Fostering Inclusivity By Linking the Implementation of Computational Simulations to Student Learning Styles — ***Ifeoluwa Babalola***, *Victor Ugaz*

3:48 Paper 186b: Incorporating Circular Economy in Chemical Engineering Education: A Multidisciplinary Approach — ***Mamoun Al-Rawashdeh***, ***Konstantinos E. Kakosimos***, *Peter Martin, Joselia Neves, Christine Schiwietz, . Savanid (Nui) Vatanasakdakul, Evren Tok,* ***Dhabia Al-Mohannadi***

4:06 Paper 186c: Modernizing Satisfaction of the ABET/Aiche Process Safety Criterion through an across-the-Curriculum Approach — ***Matthew Cooper***

4:24 Paper 186d: Implementation of Molecular Biology and Cell Line Development Courses for Future Engineers in Biopharmaceutical Industry. — ***Driss Elhanafi***

4:42: Break

5:00 Paper 186f: Chemeng Remote Experience Augmented through Technology (CREATE) Labs – Training Leaders of the Future for Industry 4.0 — ***Vijesh Bhute***, ***Umang V. Shah***, ***James I. Campbell***, *Andrew Macey, Sampad Sengupta, Pavan Inguva, Jerry Y. Y. Heng,* ***Clemens Brechtelsbauer***

5:18 Paper 186g: Providing Chemical Engineering Seniors an Industry-like Control Room Experience through a Remotely Operated Gas Permeation Experiment — ***Aravind Suresh***, *Jason Risolo, Emily Oldag*

5:36 Paper 186h: Redefining the Scale of Fluid Flow Experiments — ***Fernando Mérida Figueróa***, *Carlos Rinaldi-Ramos, Spyros Svoronos*

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(187) NSF Workshop II: Proposal Writing and Discussions with Program Managers

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, W-105A

Ram Gupta, Chair
Carole Read, Co-Chair

Sponsored by: Career Guidance Committee Liaison

3:30 Paper 187a: Proposal Writing Strategies for Fundamental Research Proposals for NSF — ***Triantafillos Mountziaris***, ***Dimitrios Papavassiliou***

4:30 Paper 187b: Interactive Breakout Panels — ***Carole Read***, *Jeanne VanBriesen, Ray Adomaitis, Shahab Shojaei-Zadeh, Steven Peretti, Mamadou Diallo*

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(188) Societal Issues in the ChE Classroom and Curriculum

Monday, Nov 14, 3:00 PM
Phoenix Convention Center, W-105C

Sindia M. Rivera-Jimenez, Chair
Sarah Wilson, Co-Chair

Sponsored by: Education

3:00: Welcoming Remarks

3:02 Paper 188a: Evidence-Based Inclusive Teaching Strategies — ***Stephanie Velegol***

3:18 Paper 188b: Increasing Accessibility for Visually Impaired STEM Students through a New Design and Rapid Prototyping Course — ***Vance Jaeger***, *Adam Stockhausen*

3:34 Paper 188c: 10 Tips to Make Your Course More Accessible and Inclusive to Disabled Students — ***Mariah Arral***

3:50 Paper 188d: Understanding Barriers to Mental Health Related Help-Seeking in Undergraduate Engineers — *Courtney Wright, Lucy Hargis, Melanie Miller, Ellen Usher, Joseph Hammer,* ***Sarah Wilson***

4:06 Paper 188e: A Diversity Index to Assess College Engineering Team Performance and Tracking Insitutional Changes on Diversity — ***Joaquin Rodriguez Alonso***, *John Keith, April A Dukes*

4:22 Paper 188f: Best Practices for the Advancement of Diversity, Equity, and Inclusion in Chemical Engineering Education — ***Reginald Rogers Jr.***, *Todd Pagano*

4:38 Paper 188g: Enhancing Chemical Engineering Identity in Young Women with a Biomedical Polymer Outreach Activity — ***Jessica Torres***, *Julie C. Liu*

4:54 Paper 188h: Why Incorporating Community and Global Issues into the Classroom Matters — *Joni Lakin, Edward W. Davis,* ***Virginia Davis***

5:10: Discussion

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(189) IDEAL Featured Session: A Conversation on Equity, Diversity, and Inclusion

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-231B

Lori McDowell, Chair
Anthony Butterfield, Co-Chair

Sponsored by: Engineering for Inclusion

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(190) Electrochemical Advances to Enable Efficient Oxygen, Hydrogen and Water Reactions II

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-232C

Ian McCrum, Chair
Hui Xu, Co-Chair
Damilola Daramola, Co-Chair
Piran Kidambi, Co-Chair

Sponsored by: Electrochemical Fundamentals

3:30 Paper 190a: Two-Dimensional Co_3O_4-Supported Metal Atoms for Water Oxidation Catalysis — ***Jingyue Liu***, *Yang Wang, Colt Murray, Timothy Delazzer*

3:45 Paper 190b: Strategically Evaluating the Stability of Antimony-Based Oxides to Design Improved Oxygen Reduction Electrocatalysts — *Melissa Kreider, Gaurav A. Kamat,* ***Michaela Burke Stevens***, *Thomas Jaramillo*

4:00 Paper 190c: Modeling the Combined Effects of Temperature, Pressure, and pH on Oxygen Evolution Thermodynamics and Kinetics — ***Ananth Govind Rajan***, *John Mark P. Martirez, Emily Carter*

4:15 Paper 190d: Accelerated Discovery of Stable and Active Materials for Oxygen Electrocatalysis — ***G. T. Kasun Kalhara Gunasooriya***

4:30 Paper 190e: A Theoretical Study on Enhanced ORR Activity and Bifunctionality of Fepc-Functionalized Graphene Via Substrate Doping, Ligand Exchange, and/or Defect Incorporation — ***Naomi Helsel***, *Pabitra Choudhury*

4:45 Paper 190h: Enhancing Electrocatalytic H_2O_2 Production Using Functionalized Carbon Catalysts — ***Brianna Ruggiero***, *Justin Notestein, Linsey Seitz*

5:00 Paper 190f: Design of High Entropy Oxides Electrocatalysts for Efficient Oxygen Evolution Reaction — ***Md Delowar Hossain***, *Jihyun Baek, Kirsten Winther, Xiaolin Zheng, Michal Bajdich*

5:15: Break

5:30 Paper 190i: Direct Electrosynthesis of Pure Aqueous H2O2 Solutions with High Production Rates Based on Carbon Catalysts Using a Solid Electrolyte — ***Yang Xia***, *Haotian Wang*

5:45 Paper 190j: Facile Glucose-Based Catalyst for Electrochemical Production of Hydrogen Peroxide — ***Xiangyu You***, *Yang Li, Fengbao Zhang, Xiaobin Fan, Wenchao Peng*

(191) Faculty Candidates in CoMSEF/Area 1a, Session 2

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-222C

Amir Haji-Akbari, Chair
Jeremy Palmer, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

3:30 Paper 191a: Energy Fingerprints for Machine Learning Prediction of Adsorption in Nanoporous Materials — ***Kaihang Shi**, Randall Snurr*

3:42 Paper 191b: Active Learning of Optimal Linear Molecular Probes to Bind with per- and Polyfluoroalkyl Substances in Water — ***Siva Dasetty**, Maximilian Topel, Yuqin Wang, Stuart J. Rowan, Sang Soo Lee, Seth B. Darling, Chris J. Benmore, Rebecca Willet, Eric Jonas, Junhong Chen, Andrew Ferguson*

3:54 Paper 191c: Leading a Way of Accurate Atomic-Scale Understanding of Materials and Interfaces By Interface Force Field — ***Cheng Zhu***

4:06 Paper 191d: Accelerated Prediction of Metal–Organic Framework Electronic Properties Via High-Throughput Quantum-Chemical Calculations and Machine Learning — ***Andrew Rosen**, Justin Notestein, Randall Snurr*

4:18 Paper 191e: Block Copolymer Blending Strategy for Creating Alternating Gyroid Morphology — ***Sojung Park**, Frank S. Bates, Kevin D. Dorfman*

4:30 Paper 191f: Plasmonic Response of Nanoparticle Assemblies — ***Zachary Sherman**, Manuel Dominguez, Kihoon Kim, Jiho Kang, Stephanie A. Valenzuela, Murari Singh, Emily Lin, Eric V. Anslyn, Delia Milliron, Thomas Truskett*

4:42 Paper 191g: Machine-Learned Committor Functions for Reactive Molecular Dynamics — ***Jacob Gissinger**, Kristopher Wise*

4:54 Paper 191h: Bridging Thermal and Electrochemical Catalysis: Rational Catalyst Design at Atomic Scales — ***Shyam Deo***

5:06 Paper 191i: Accelerating the Design of Single-Site Materials for Catalysis Using Computational Data, Experimental Data, and Machine Learning — ***Aditya Nandy**, Heather Kulik*

5:18 Paper 191j: Progress in the Understanding of Chemical Interactions through Atomic Scale Modeling – Applications in Catalyst Design — ***Joakim Halldin Stenlid, PhD***

5:30 Paper 191k: Transfer Learning of Graph Neural Networks As a General Approach to Accelerate Computational Catalysis Modeling — ***Tian Tian**, Adeesh Kolluru, Joseph Musielewicz, Janghoon Ock, Zachary Ulissi*

5:42 Paper 191l: Integrating Computational Reaction Discovery in the *Ab Initio* Nanoreactor with Kinetic Modeling and Sensitivity Analysis — ***Rui Xu**, Jan Meisner, Alexander M. Chang, Keiran C. Thompson, Todd J. Martinez*

5:54 Paper 191m: Developing of Theoretical Methods for Multi-Metallic Alloys — ***Shikha Saini***

(192) Molecular Simulation and Modeling of Complex Molecules

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-223

Yamil Colón, Chair
Peng Bai, Co-Chair
Abhishek Sharma, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

3:30 Paper 192a: Stabilizing Network Phases By Blending of LAM and Cyl Forming High-χ Block Oligomers — ***J. Ilja Siepmann**, Zhengyuan Shen, Ke Luo, Daoyuan Li, Mahesh Mahanthappa, Timothy P. Lodge*

3:45 Paper 192b: Effect of Chain Dynamics on the Free Volume Elements of Glassy Polymers from Atomistic Molecular Dynamics Simulations — ***Mohammed Al Otmi**, Janani Sampath*

4:00 Paper 192c: Effect of Zwitterionic Molecules on Solvation and Transport of Sodium and Potassium Cations in Ethylene Oxide-Based Electrolytes — ***Manh Tien Nguyen**, Qing Shao*

4:15 Paper 192d: Hydrophobic Base Pair Stacking As the Main Stabilizer for Double Helix Structure of DNA: A Molecular Modeling Approach — ***Arthur Gonzales III**, Alexis Azucena*

4:30 Paper 192e: Shapes and Thermodynamics of Membranes with Boundaries — ***Kevin S. Silmore**, James W. Swan*

4:45 Paper 192f: Molecular Models to Assess Barrier Properties of Bacterial Cell Walls — *Rakesh Vaiwala, Pradyumn Sharma,* ***Ganapathy Ayappa***

5:00 Paper 192g: Combined Molecular Dynamics and Neural Network for Predicting Lanthanide Selective Binding Activity of Lbt Peptides — ***Yiming Wang**, Dr. Kathleen J. Stebe, Ravi Radhakrishnan*

5:15 Paper 192h: Toward Wide-Spectrum Antivirals Against Coronaviruses: Modeling the Binding Mechanisms of Repurposed Drugs to the Sars-Cov-2 RNA-Dependent RNA Polymerase — ***Fabian Byléhn**, Cintia Menéndez, Gustavo Perez-Lemus, Walter Alvarado, Juan De Pablo*

5:30 Paper 192i: Free Energy Landscapes for Elucidating the Structural Consequences of Exon-20 Mutations on the ErbB Family of Protein Kinases — ***Ashwin Ravichandran**, Chang Woon Jang, Mohit Mehta, Daniel J. Kozuch, John W. Lawson*

5:45 Paper 192j: Computational and Fourier-Transform Infrared Spectroscopy Study of Chemical Composition and Its Effect on Asphalt Aging — ***Emmy Huang**, Fazlur Rahman, Sagar Ghos, Musharraf Zaman, Edgar A. O'Rear III, Liangliang Huang*

(193) Advanced Treatment Technologies for Water II

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-225A

Steven Weinman, Chair
Selma Mededovic, Co-Chair
Deepak Sharma, Co-Chair

Sponsored by: Water

3:30 Paper 193a: Novel Sorbents Development for Selective Removal of Pfas from Gaseous Phase and Aqueous Stream — ***Maoqi Feng***

3:55 Paper 193b: A Silica-Based Approach to Remove Valuable Components from Produced Water — ***Songpei Xie**, Michael Miranda, Anirban Ghosh, Madelyn Shaw, Mark Krzmarzick, Dave Lampert, Clint Aichele*

4:20 Paper 193c: Improving Electrode Performance By Engineering *Shewanella Oneidensis* MR1 — ***Jiacheng Zhou**, Gregg P. Kotchey, David V. P. Sanchez, Seok Hoon Hong*

4:45 Paper 193d: Facile Hydrothermal Synthesis of Ferrites and Ferrite/Graphene Nanocomposites for the Catalytic Degradation of Organic Pollutants in Water — ***Marjorie Lara Baynosa**, Amr Hussein Mady, Jae-Jin Shim*

5:10 Paper 193e: Extractive Crystallization Calcium Acetate Deicer from Water Plant Residuals — ***Alexander Mathews**, Samuel Degife*

5:35 Paper 193f: Adsorption of Pfas By Zeolites — ***Charles Ponge**, David R. Corbin, Mark B. Shiflett*

(194) Atmospheric Chemistry and Physics: Laboratory Studies

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-225B

Denis Sarigiannis, Chair
Marwa El-Sayed, Co-Chair

Sponsored by: Air

3:30 Paper 194a: Effect of Combustion Particle Morphology on Biological Responses in a Co-Culture of Human Lung Epithelial and Macrophage-like Cells — ***Kerry Kelly**, Kamaljeet Kaur, Raziye Mohammadpour, Hamid Ghandehari, Robert Paine, Christopher Reilly*

3:55 Paper 194b: Using Low-Cost Air Purification to Mitigate COVID-19 Transmission in Schools and Community Settings — *William Gasparrini,* ***Kristina Wagstrom***

4:20 Paper 194c: Hybrid Water Activity – a Novel Framework for CCN Analysis of Sparingly Water Soluble Organic Aerosols — ***Kanishk Gohil***, *Chun-Ning Mao, Dewansh Rostogi, Chao Peng, Mingjin Tang, Akua Asa-Awuku*

4:45 Paper 194d: Combined Ice Crystal Growth Chamber and Flow System to Investigate Atmospheric Secondary Ice Nucleation — ***Sylvia Sullivan***

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(195) Integrated Biorefineries: Technologies and TEA/LCA

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, W-103A

Rajesh Shende, Chair
Ram Gupta, Co-Chair
Sandeep Kumar, Co-Chair

Sponsored by: Fuels and Petrochemicals Division

3:30 Paper 195a: Building a Toolbox for Integrating Economic and Environmental Performance of Bio-Based Products — ***Samir Meramo***, *Peter Fantke, Sumesh Sukumara*

4:00 Paper 195b: Enhanced Sugar Yield from Cellulose By Ammonium Salt Based Pretreatment — *Monidipa Bose,* ***Eshita Saha****, Shyamal Roy*

4:07 Paper 195c: TEA and LCA of Renewable Hydrocarbon Fuels and Co-Products from Lignocellulosic Biomass Via 2,3 Bdo Fermentation, Separation, Dehydration and Oligomerization. — ***Marco Avendano***, *Qiang Fu, Jianpei Lao, Oindrila Gupta, Mi Lu, Sankar Nair, Matthew Realff*

4:37 Paper 195d: Advanced Biorefinery Feedstocks from Waste Biomass: Technoeconomic Assessment of Integrated Air Classification-Hydrothermal Carbonization-Pelletization Processes — ***Md Tahmid Islam***, *Nepu Saha, Jordan Klinger, Toufiq Reza*

5:07 Paper 195e: Kinetic Modeling of the Acetone–Butanol–Ethanol Fermentation of Eucalyptus Wood-Derived Xylose By Clostridium Beijerinckii NCIMB 8052 — ***Elmer Ccopa Rivera***, *Hyun Kwon, Thaddeus Ezeji, Rubens Maciel Filho, Adriano P. Mariano*

5:14 Paper 195f: Oxidative Fast Pyrolysis of Groundnut Shell (GNS) in the Catalytic and Non-Catalytic Mode for Biofuel Production — ***Geeta Kumari***, *Bhavin Soni*

5:21 Paper 195g: TEA/LCA of Integrated Biochemical and Hydrothermal Processing of Corn Stover for Fuels and High Value Products — ***Bharathkiran Maddipudi***, *Khang Huynh, Vinod S. Amar, Katelyn Shell, Anuj Thakkar, Anuradha Shende, Sergio Hernandez, John E. Aston, Sandeep Kumar, Ram Gupta, Rajesh Shende*

5:51 Paper 195h: Production of Biodiesel from Waste Cooking Oil — ***Kareem Tharwat Sr.***

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(196) Ionic Liquids: Novel Separation, Catalytic reaction and Electrochemical Processes

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-228B

Kevin West, Chair
Brooks Rabideau, Co-Chair
Tugba Turnaoglu, Co-Chair
Xiangping Zhang, Co-Chair
Feng Huo, Co-Chair

Sponsored by: Green Process and Product Engineering

3:30 Paper 196a: Multiscale Inverse Design of High-Performance Ionic Liquid Solvents for High-GWP Refrigerant Separation — ***Mohammed Sadaf Monjur***, *Ashfaq Iftakher, M M Faruque Hasan*

3:44 Paper 196b: Measuring Henry's Law Constants and Infinite Dilution Activity Coefficients of Gases and Liquids in Ionic Liquids Using Gas Chromatography for Olefin/Paraffin Separations — ***Kimberly Bourland***, *Joan Brennecke*

3:58 Paper 196c: New Dimensions in Fabricating Ionic Polymers of Intrinsic Microporosity for Advanced Membrane Gas Separation — ***Shuangjiang Luo***, *Wei Xie, Zhili Cai, Can Wang, Peijun Zheng*

4:12 Paper 196d: Ionic Liquids Based Membranes for Gas Separation — ***Lu Bai***

4:26 Paper 196e: Efficient Fixation of CO_2 into Cyclic Carbonate Catalyzed By Ionic Liquids in Microchannels — ***Feng Huo***, *Yu Chen, Jiayuan Yu, Yiqian Yang, Chunshan Li*

4:40 Paper 196f: Structural Reorganization of Ionic Liquid Electrolytes By Charge/Discharge Circle — ***Kun Zhang***, *Guohui Zhou, Timing Fang, Xiaomin Liu*

4:54 Paper 196g: Synthesis, Characterization, and Assembly of All Polyelectrolyte Diblock Copolymers from Poly (ionic liquid) and Weak Polyelectrolyte Blocks — ***Kayla Foley***, *Keisha Walters*

5:08: Break

5:22 Paper 196i: Dynamic and Structural Properties of Ionic Liquid Electrolytes — ***Jiahuan Tong***, *Feng Huo, Bilin Zhuang, Suojiang Zhang, Xiaodong Liang, Nicolas von Solms*

5:36 Paper 196j: Highly Dispersed Ionic Liquids in Mesoporous Molecular Sieves Enable a Record NH_3 Absorption — ***Zhiyong Li***

5:50 Paper 196k: Rare-Earth Separation Based on the Differences of Ionic Magnetic Moment Via Quasi-Liquid Strategy — ***Fujian Li***

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(197) Informing Policy - Climate Solutions Policy Initiative (CSPI)

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-127A

John Cirucci, Chair
Martin Abraham, Co-Chair

Sponsored by: Public Affairs and Information Committee (PAIC)

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(198) Transitioning from Your Academic Career to Your Future as a Professional (Panel Discussion)

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-231C

Cory Thomas, Chair

Sponsored by: Young Professionals Committee (YPC)

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(199) Role of Chemical Engineers in Non-Traditional Industries

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, W-102B

Dhaval Bhandari, Chair

Sponsored by: Management Division

3:30 Paper 199a: Impact of Environmental Regulatory Compliance: Corporate Responsibility and Economic Consequences — ***Rengasamy Kasinathan***, *Madalyn Bozinski*

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(200) Fibers and Coatings: 1D and 2D Composites

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-121B

Enoch Nagelli, Chair
Crystal Owens, Co-Chair
Luyi Sun, Co-Chair

Sponsored by: Composites

3:30 Paper 200a: Composite Fibers with Layered Structures for Structural and Smart Applications — *Weiheng Xu,* ***Kenan Song***

3:45 Paper 200b: 1D Porous Fibers Via a New Spinning Method — ***Mohammed Bawareth***, *Kenan Song*

4:00 Paper 200c: Encapsulation of Nanoscale Organic Hybrid Materials and Metal-Organic Frameworks in Electrospun Polymer/Ceramic Fibers for Direct Air Capture of CO_2 — ***Kyle Kersey***

4:15 Paper 200d: Electromagnetic Interference Shielding Performance of $Ti_3C_2T_x$ Mxene/Polyelectrolyte Fibers and Composite Laminates — ***Farivash Gholamirad***, *Nader Taheri-Qazvini*

4:30 Paper 200e: Temperature Responsive PBT Bicomponent Fibers for Dynamic Thermal Insulation — ***Ninad Khadse***, *Jay Park*

4:45 Paper 200f: The Continuous Millifluidic Surface Modification of Silver Nanowires By Palladium Via Galvanic Replacement Reaction — ***Destiny Williams***, *Shohreh Hemmati, James Smay*

5:00 Paper 200g: Fabrication and Characterization of Wool Textile-Based Supercapacitors — *Mona Bavarian, **Alyssa Grube***

5:15 Paper 200h: Physical Blending to Produce Chitosan, PLA, and PCL-Based Composite Films for Biomedical Applications — ***Ali Alshami**, Abdulrahman Al-Shami*

5:30: Break

5:45 Paper 200j: MOF Integrated 3D Self-Supported Aerogels Constructed *Via* Solid Templating of Electrospun Nanofibers — ***Vahid Rahmanian**, Tahira Pirzada, Saad A. Khan*

(201) Carbon Nanomaterials II: Dispersion, Surface Structure, and Biointeractions

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, W-104B

Anju Gupta, Chair

Sponsored by: Carbon Nanomaterials

3:30 Paper 201a: 2D Diamond Superstructures in Interlayer-Bonded Twisted Bilayer Graphene: Mechanical Response and Thermal Transport from Molecular-Dynamics Simulations — *Mengxi Chen, Afnan Mostafa, **Asanka Weerasinghe**, Andre R. Muniz, Ashwin Ramasubramaniam, Dimitrios Maroudas*

3:55 Paper 201b: Carbon Nanotube Length Reduction from Planetary Ball Milling — ***Mason Rhue**, Brian Grady*

4:20 Paper 201c: Porosity and Crystallinity Dynamics of Carbon Black during Internal and Surface Oxidation — ***Georgios Kelesidis**, Nicola Rossi, Sotiris E. Pratsinis*

4:45 Paper 201d: Automated and High Precision Measurement of Carbon Nanotube (n,m) Dependent Extraction Conditions in Aqueous Two Phase Extraction — *Christopher Sims, **Jeffrey Fagan***

5:10 Paper 201e: Divalent Metal Cation Optical Sensing Using Single-Walled Carbon Nanotube Corona Phase Molecular Recognition — ***Xun Gong**, Sooyeon Cho, Michael Strano*

5:35 Paper 201f: Synthesis and Application of Glycopolymer-Wrapped Carbon Nanotubes for Detecting Carbohydrate-Protein Interactions — *Ana DiLillo, Ka Keung Chan, Xue-Long Sun, **Geyou Ao***

(202) Nanomaterials for Energy Conversion

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, W-104A

Tae-Sik Oh, Chair
Seung Soon Jang, Co-Chair

Sponsored by: Nanomaterials for Energy Applications

3:30 Paper 202a: Machine Learning Approach to First-Principles Database for Designing Active Nanomaterials for Electrochemical Energy Convergence — ***Byungchan Han**, Hoje Chun, Minjoon Hong*

4:05 Paper 202b: Modulating the Active Sites of Metal–Nitrogen–Doped Carbon Catalysts By Orbital Coupling for Highly Active and Selective CO_2 Electrochemical Reduction — ***Jeong Woo Han***

4:40 Paper 202c: *Sp-D* Orbital Hybridization Driven Metal-Graphene and Metal-Graphene-Metal Catalyst for Direct and Electrochemical Synthesis of Hcooh from CO_2: First-Principles Approach — ***Jinwon Cho**, Ji Il Choi, Matthew Drexler, Faisal M. Alamgir, Seung Soon Jang*

5:00 Paper 202d: High-Temperature Flow Synthesis of Lead Halide Perovskite Nanocrystals — *Kameel Abdel-Latif, **Fazel Bateni**, Mahdi Ramezani, Milad Abolhasani*

5:20 Paper 202e: Photo-Catalyzed Polymerization of Substituted Anilines Via Psi Active Sites — ***Marc Nabhan**, G. Kane Jennings, David Cliffel, Tyler Oddo*

5:40 Paper 202f: Kinetic Control of Intrinsic Pores in Monolayer Graphene for Large-Area Proton Selective Membranes — ***Piran Kidambi***

(203) Analyses of Mixing Processes in Bioreactors

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-227C

Matthew Flamm, Chair
Navraj Hanspal, Co-Chair

Sponsored by: North American Mixing Forum

3:30 Paper 203a: Flow Simulation of Bioreactors Using Entropic Lattice Boltzmann Method — *Sai Nithin Reddy Adidela, **Chakradhar Thantanapally**, **Vinay Kariwala**, Salvatore Arcidiacono, Santosh Ansumali*

3:55 Paper 203b: Predicting the Effect of Gradients on Cell Culture Performance in Large Scale Bioreactors — ***Katherine Raudenbush**, John Thomas, Marianthi Ierapetritou*

4:20 Paper 203c: Fluid-Dynamic Simulation of a Flat-Panel Bioreactor with Emphasis on Mixing, Mass Transfer and Inorganic CO_2 Chemistry — ***John Parra-Alvarez**, Mauro Lua, Lieve Laurens, Hari Sitaraman, Jonathan Stickel, Heinnickel Mark, Paddock Troy*

4:45 Paper 203d: Comparison of Modeling Methodologies for Simulating a Gassed-Agitation System with Experimental Validation — ***Christopher Tyler**, John Thomas*

5:10 Paper 203e: Geometrical Optimization of Side-Entry Propeller Designs for the Homogenization Process in Biogas Fermenters — ***Markus Kolano**, Matthias Kraume*

5:35 Paper 203f: Multiphysics Simulation of an Internal Loop Airlift Photobioreactor for Microalgae Cultivation — ***Lifeng Li**, Zulfida Mohamad Hafis Mohd Shafie, Ting-Yi Huang, Raymond Lau, **Chi-Hwa Wang***

(204) Fluidization: Modeling

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, W-106C

Chris Boyce, Chair
Peter Blaser, Co-Chair

Sponsored by: Fluidization and Fluid-Particle Systems

3:30 Paper 204a: A Critical Assessment of the Energy Minimization Multi-Scale (EMMS) Model for Turbulent Fluidized Beds — ***Pedram Pakseresht**, Jesse Capecelatro, Yuan Yao, Yi Fan, Jorg Theuerkauf, Lennard Lindmuller, Stefan Heinrich*

3:45 Paper 204b: A New Model for Liquid Bridges in Wet Particles in Fluidisation — *Ning Yang, Leina Hua, **Raffaella Ocone***

4:00 Paper 204c: Comparison of Coarse-Grained CFD-DEM and KTGF Simulation for Industry Scale Fluidized Beds — ***Thomas Eppinger**, Ravindra Aglave*

4:15 Paper 204d: Concentric-Tube Internal Loop Airlift Reactors for Microalgae Cultivation: A Review — ***Lifeng Li**, Xiaoyun Xu, Wujun Wang, Raymond Lau, **Chi-Hwa Wang***

4:30 Paper 204e: Model Parameters Calibration for DEM By Macroscopic Characterization of Granular Material — ***Filip Francqui**, Salvatore Pillitteri, Aurelien Neveu, Geoffroy Lumay*

4:45 Paper 204f: Heat and Mass Transfer within Dynamically Structured Bubbling Fluidized Beds Subject to Vibration: A Two-Fluid Modeling Study — ***Qiang Guo**, Shawn Chiu, Wei Da, Chris Boyce*

(205) Novel Nanoparticles and Nanostructured Catalysis for Energy and Environmental Applications

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, W-106A

Timothy Brenza, Chair

Sponsored by: Nanoparticles

3:30 Paper 205a: Computationally Guided Design of Ferrite Nanoparticles for Magnetic Inductive Heating — ***Venkata Rohit Punyapu**, Rachel Getman*

3:48 Paper 205b: Mixing Immiscible Elements to Create a Library of Single Phase Ceramic Nanoparticles By Continuous Flame Synthesis — ***Shuo Liu**, Chaochao Dun, Jilun Wei, Jeffrey J. Urban, Mark Swihart*

4:06 Paper 205c: Preparation of Large-Pore-Volume Al_2O_3 Microspheres As Catalyst Support Via Microfluidics — ***Huilin Yi***, *Yujun Wang, Guangsheng Luo*

4:24 Paper 205d: Dial-a-Material: Precise Manufacturing Technology for Bimetallic and Monometallic Nanoparticles — ***Bruno Pinho***, *Laura Torrente-Murciano*

4:42 Paper 205e: Development of Green Roofing Tiles with the Use of Novel Photocatalytic and Reflective TiO_2 Nanoparticles — ***Maria Kouroutzi***, *Antonios Stratidakis, Marianthi Kermenidou, Katerina Karatisoglou, Vasilios Kakoutopoulos, Agis Kothalis, Spyros Karakitsios, Dimosthenis Sarigiannis*

5:00 Paper 205f: Gas Phase Coating of Fluidized Particles: Towards Ton-Scale Production with Nano-Precision — ***J Ruud Van Ommen***

5:18 Paper 205g: Flame Aerosol Synthesis of High-Entropy Ceramic Nanoparticles — ***Shuo Liu***, *Chaochao Dun, Jilun Wei, Jeffrey J. Urban, Mark Swihart*

5:36 Paper 205h: Filtration of NaCl Aerosols Using Porous Versus Non-Porous Filter Media — ***Amulya Poudyal***

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(206) Particulate Systems: Dynamics and Modeling: Discrete/Continuum Models

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, W-106B

Maria Tomassone, Chair
Bhaumik Bheda, Co-Chair

Sponsored by: Solids Flow, Handling and Processing

3:30 Paper 206a: Impregnation of Catalyst: Batch and Continuum Processes — ***Maria Tomassone***, *William Borghard*

3:48 Paper 206b: DEM and Experimental Comparison of Particle Heat Transfer and Geometry Driven Particle Flow Patterns — *Jason Schirck,* ***Aaron Morris***, *Korey Cook, Zhiwen Ma*

4:06 Paper 206c: Effect of Mechanical Interlocking on Particle-Phase Stress in Sheared Granular Flows — ***Elizabeth Suehr***, *Jiecheng Yang, Jennifer Curtis*

4:24 Paper 206d: Continuum Modeling of Cohesive Powder Flow — ***Sameer Kamath***, *Sean Garner, Marcial Gonzalez, William Ketterhagen, Carl R. Wassgren*

4:42 Paper 206e: Simulation of Particle Dissolution Using the Geometrical Phase Field Approach — *Dominik Sleziona, David Ely,* ***Markus Thommes***

5:00 Paper 206f: DEM Study of a Vibrational Powder Transport System — ***Martina Trogrlic, MSc***, *Dalibor Jajcevic, Johannes G. Khinast, Pankaj Doshi, Barry Ager, Tata Venkata, Stephen Franklin, David Barling*

5:18 Paper 206g: Multiscale Computational Fluid Dynamics Method for Slug Flow Reactor Simulation — ***Shin Hyuk Kim***, *Moo Sun Hong, Jay H. Lee, Richard D. Braatz*

5:36 Paper 206h: Effect of Particle Shape on Deposition Behavior in Cascade Impactor — ***Ryosuke Mitani***, *Shuji Ohsaki, Hideya Nakamura, Satoru Watano*

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(207) Control Strategies in Pharmaceutical Development and Manufacturing II

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-122C

Shujauddin Changi, Chair
Christopher Marton, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

3:30 Paper 207a: Mechanistic Study of Diketopiperazine Formation during Solid Phase Peptide Synthesis of Tirzepatide — ***Jingyao Wang***, *Mark Berglund, Fareed Sayyed, Matthew C. Embry, Stephen Groskreutz, Martin Johnson, Timothy M. Braden, Michael Kopach*

3:51 Paper 207b: Strategies for Mitigation and Control of PS80 Degradation in a Monoclonal Antibody Downstream Process — *Kevin Chang,* ***Hope McMahon***, *Zifan Gong, Andreas Sophocleous, Robert Luo, Antonio Ubiera*

4:12 Paper 207c: Eliminating Batch-to-Batch Variability in Monoclonal Antibody Production Using Closed-Loop Control — ***Thomas Kavanagh***, *Maria Papathanasiou, Cleo Kontoravdi*

4:33 Paper 207d: Systematic Control Strategy Development for a Continuous Direct Compaction Line Via the Control Strategy Evaluation Tool (CET) — ***Jakob Rehrl***, *Julia Kruisz, Selma Celikovic, Peter Toson, Dalibor Jajcevic, Johan Remmelgas, Thomas O'Connor, Abdollah Koolivand, Geng Tian, Scott M. Krull, Johannes G. Khinast*

4:54 Paper 207e: Modeling, Simulation and Control of Twin-Screw-Granulation and Fluid-Bed-Drying Applied to a ConsiGma™-25 Line — ***Selma Celikovic***, *Jakob Rehrl, Johannes Poms, Martin Horn, Johannes G. Khinast*

5:15 Paper 207g: A Knowledge-Guided Framework for the Effective Application of Machine Learning Models in the Development of Condition Monitoring Systems. — ***Rexonni Lagare***, *Yan-Shu Huang, Zoltan Nagy, Gintaras Reklaitis*

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(208) Enabling Technologies: Mechanistic and statistical modeling

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-123

Neil C. Dalvie, Chair
Rachel Bade, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

3:30 Paper 208a: *In silico* Design of a Commercial-Scale Bioreactor for Optimum Oxygen Transport Using Computational Fluid Dynamics (CFD) — *Iman Mirzaee, Mark Brothers, Gregory Stimpfl,* ***Saeed Jafari Kang***, *Maryam Medghalchi, Fabrice Schlegel, Pablo A. Rolandi*

3:51 Paper 208b: Automated Reaction Optimization Under Dynamic Flow Conditions — ***Brian Wyvratt***, *Jonathan P. McMullen*

4:12 Paper 208c: Self-Supervised Learning Methods for Drug Substance and Drug Product Characterization in the Pharmaceutical Industry — ***Hossein Salami***, *Daniel Skomski*

4:33 Paper 208d: Development of a High-Throughput Kinetics Protocol and Applications — ***Xiao Li***, *Anna Dunn, Robert Yule, Boung Wook Lee*

4:54 Paper 208e: A Techno-Economic Assessment of Acrylates Downstream Processing with Membrane Extraction — ***Jie Yang***, *Anita Buekenhoudt, Miet Van Dael, Patricia Luis, Yamini Satyawali, Robert Malina, Sebastien Lizin*

5:15 Paper 208f: Evaluating the Syringeability of Drug Products Using Mechanistic in-Silico Modeling — ***Saman Seifi***, *Calvin Clark, Leonela Vega Loaisa, Fabrice Schlegel, Dan Groszmann, Pablo A. Rolandi*

5:36 Paper 208g: Digital Design and Evaluation of Separation Alternatives for the Green Manufacturing of Lomustine — ***Daniel Casas Orozco***, *Daniel Laky, Jaron Mackey, Varun Sundarkumar, Giulia Murbach De Oliveira, David H. Thompson, Gintaras Reklaitis, Zoltan Nagy*

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(209) Special Session In Honor of Dr Muthanna H. Al-Dahhan's 65th Birthday (Invited Talks)

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-222A

Shaibal Roy, Chair

Sponsored by: Process Development Division

3:30 Paper 209a: Sustainable Process Development – a Corporate Perspective — ***Shaibal Roy***

3:55 Paper 209b: Pairing experimental and mathematical modelling approaches for the development of highly predictive multiphase flow systems models — ***Sebastian Uribe***, *Muthanna Al-Dahhan*

4:20 Paper 209c: Invited Paper - Patrick L. Mills — ***Patrick Mills***

4:45 Paper 209d: Hydrogen production by enhanced methane decomposition over Co-Rh bimetallic catalyst — ***Mohammed Al Mesfer***, *Mumtaj Shah, Mohd Danish*

5:10 Paper 209e: A Novel Position Reconstruction Algorithm for Particle Tracking Based on the Finite Element Method (FEM) — *Ghazaleh Mirakhori,* ***Jamal Chaouki****, Bruno Blais, Jocelyn Doucet*

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(210) Regenerative Engineering Society III

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-121A

Kristin Morgan, Chair

Sponsored by: Regenerative Engineering Society

3:30 Paper 210a: Physical Implications of Therapy Induced Senescence and Polyploidy in an Evolving Tumor Microenvironment — ***Michelle R. Dawson***

4:10 Paper 210b: Presentation Title - Pending — ***Karl Lewis***

4:50 Paper 210c: Smart Hydrogels for Regenerative Engineering — ***Nicholas Peppas***

5:30 Paper 210d: Engineering the Bio/Nano Interface for Targeted Modulation of the Immune System — ***Evan Scott***

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(211) Area Plenary: Adsorption and Ion Exchange - In Honor of Prof. Andreas Seidel-Morgenstern (Invited Talks)

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-131C

F Handan Tezel, Chair
Daniel Siderius, Co-Chair

Sponsored by: Adsorption and Ion Exchange

3:30: Welcoming Remarks

3:36 Paper 211a: Determination of Pure and Binary Adsorption Isotherms Using Concentration Pulse Chromatography — ***F Handan Tezel***

3:54 Paper 211b: Advances in the characterization of porous materials for applications in chromatography — *Carola Schlumberger, Carlos Cuadrado Collados, Jakob Söllner,* ***Matthias Thommes***

4:12 Paper 211c: Towards Preparative Chromatographic Classification of Polydisperse Products — ***Malte Kaspereit****, Malvina Supper*

4:30 Paper 211d: Simulated Moving Bed Reactor for Enhancing the Productivity of Equilibrium Limited Reactions — ***Balamurali Sreedhar****, Megan E. Donaldson*

4:48 Paper 211e: Engineering tools for screening and discovery of solid sorbents for CO2 capture — ***Arvind Rajendran***

5:06 Paper 211f: Optimising adsorption-desorption cycles with flexible Metal Organic Frameworks — *Rahul Maity, Mohsen Gholami,* ***Joeri Denayer***

5:24 Paper 211g: Selective Adsorption of Surfactants on Coronavirus Virions — ***Alexander Neimark****, Kolattukudy Santo*

5:42 Paper 211h: CORE-SHELL AND ENCAPSULATED ADSORBENTS FOR FLOW THROUGH PURIFICATION OF LARGE BIOMOLECULES AND NANOPARTICLES — ***Giorgio Carta***

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(212) Developments in Extractive Separations: Processes

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-132A

David Cantu, Chair
George S. Goff, Co-Chair

Sponsored by: Extractions

3:30 Paper 212a: Taylor-Couette Flow and Multiphase Operations — ***Georg Rudelstorfer****, Rafaela Greil, Maximilian Neubauer, Annika Grafschafter, Matthaeus Siebenhofer, Susanne Lux*

3:48 Paper 212b: Separation of Azeotropic Refrigerant Mixtures Using Extractive Distillation with Ionic Liquid Entrainers — *Ethan A. Finberg,* ***Mark B. Shiflett***

4:06 Paper 212c: Antagonistic Role of Aqueous Complexation in the Solvent Extraction and Separation of Rare Earth Ions — ***Pan Sun****, Erik A. Binter, Zhu Liang, M. Alex Brown, Artem V. Gelis, Ilan Benjamin, Mrinal Bera, Binhua Lin, Wei Bu, Mark Schlossman*

4:24 Paper 212d: Continuous Millifluidic Liquid-Liquid Extraction: Digital Design and Development — ***Jaron Mackey****, Devna Grover, Gabriella Pruneda, Zoltan Nagy*

4:42 Paper 212e: The Development of Structured Ligands and CO_2-Facilitated Hydrometallurgy to Extract Critical Elements from Unconventional Resources — *Hunter Vibbert,* ***Whai Shin Ooi****, Seokyoon Moon, Ah-Hyung Alissa Park*

5:00 Paper 212f: Sustainable Recovery of Butyric Acid through Salt-Induced Aqueous Two-Phase Extraction Using Non-Ionic Surfactants — ***Kristel Gatdula****, William Holmes, Emmanuel Revellame*

5:18 Paper 212g: Greener Extraction of Rare Earth Elements from Coal Fly Ash — ***Cesar Martinez Bejarano****, Yasaman Ghanbari, Kenneth Walker, April Wright, Isaiah Morones, Sergio Martinez-Monteagudo, Catherine Brewer*

5:36 Paper 212h: Oil Recovery from Produced Water Via Selective Oil Filtration — ***Carolyn Cooper****, Frank Seibert, Kerry Kinney, Lynn E. Katz*

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(213) Honorary Session for Prof. Suzana Nunes I

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-131B

Dibakar Bhattacharyya, Chair
Isabel Escobar, Co-Chair
Lakshmeesha Upadhyaya, Co-Chair
Cristiana Boi, Co-Chair

Sponsored by: Membrane-Based Separations

3:30 Paper 213a: Introduction and Opening Remarks — ***Dibakar Bhattacharyya, Isabel Escobar, Cristiana Boi, Lakshmeesha Upadhyaya***

3:40 Paper 213b: Snips Membranes-How It Came about — ***Klaus Peinemann***

4:00 Paper 213c: Sustainable Production of Nanoemulsions By Membrane Emulsification for Biomedical and Bioprocessing Applications — *Usman Syed,* ***Joao Crespo****, Carla Brazinha*

4:20 Paper 213d: Rational Design of DNA-Based Responsive Membranes — ***Thomas Schäfer***

4:40 Paper 213e: Integrating Biological Functions in Artificial Membranes — ***Lidietta Giorno***

5:00 Paper 213f: Artificial Water Channels-Toward Biomimetic Membranes for Desalination — ***Mihail Barboiu***

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(214) Plenary Session: Crystallization and Evaporation - Area 2B (Invited Talks)

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-131A

Thomas Vetter, Chair
Christopher L. Burcham, Co-Chair

Sponsored by: Crystallization and Evaporation

3:30: Welcoming Remarks

3:35 Paper : Effects of Fluid Flow on Primary and Secondary Nucleation in Crystallization Processes — ***Jan Sefcik***

4:25: Discussion

4:35 Paper 646a: Simultaneous Lattice Incorporation and Co-Precipitation of Impurities in Solution Crystallization — ***Fredrik Nordstrom****, Qi Jiang, Tommasina Bramante, Mitchell Paolello, Joseph Kratz, James Geier, Michael Toresco, Kayla Bensley,* ***Gerard Capellades***

5:03 Paper 341b: Nonclassical Mechanisms to Irreversibly Suppress β-Hematin Crystal Growth — ***Peter Vekilov****, Wenchuan Ma, Victoria Balta, David Sullivan, Jeffrey Rimer*

5:31 Paper 148a: Crystal Morphology Prediction: An Alternative Framework Via Kmc — ***Tobias Mazal****, Michael F. Doherty*

5:59: Concluding Remarks

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(215) Feedstock Conversion Interface Consortium – Understanding Feedstock Variability to Enable Next Generation Biorefineries (Invited Talks)

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-226B

Edward Wolfrum, Chair
Vicki Thompson, Co-Chair

Sponsored by: Sustainable Biorefineries

3:30 Paper 215a: Multiphysics-Resolved Digital Twins of Feedstock Preprocessing and Handling Unit Operations: Recent Progress and Best Practices — ***Yidong Xia***, *Wencheng Jin, Ahmed Hamed, Jordan Klinger, Nepu Saha, Tiasha Bhattacharjee, Vicki Thompson, C. Luke Williams, David Thompson, Lynn Wendt*

3:49 Paper 215b: Quantitative Study of Particle Attributes Effect on the Permeability and Reactor Scale-up in a Flow-through Packed Bed Processing of Lignocellulosic Biomass — ***Yudong Li***, *Matan Lieber-Kotz, Xiaowen Chen, David A. Sievers*

4:08 Paper 215c: Leveraging Advanced Imaging and Computational Techniques for Characterizing Biomass Feedstock Transport Properties — ***Meagan Crowley***, *Hari Sitaraman, Jordan Klinger, Francois Usseglio Viretta, Nicholas E. Thornburg, Nicholas Brunhart-Lupo, Michael Pecha, Jim Dooley, Yidong Xia, Peter N. Ciesielski*

4:27 Paper 215d: *Mitigating Risks of Feedstock Variability on Low-Temperature Conversion Processes* — ***Philip Laible***, *James Gardner, Davinia Salvachua, Jeffrey Linger, Peter Larsen, Xiaowen Chen, Jacob S. Kruger*

4:46 Paper 215e: Mechanical and Flow Characterization of Loblolly Pine Residues — ***Jordan Klinger***, *Tiasha Bhattacharjee, Nepu Saha, Susan Carilli, Noah Berglund, Wencheng Jin, Yidong Xia*

5:05 Paper 215f: Continuum-Mechanics-Based Flow Modeling of Particulate Milled Biomass — ***Wencheng Jin***, *Yimin Lu, Jordan Klinger, Yidong Xia*

5:24 Paper 215g: Scale-up of Corn Stover Comminution Population Balance in Knife Mills — ***Tiasha Bhattacharjee***, *Jordan Klinger, Vicki Thompson, Yidong Xia, Susan Carilli, Monica Oliva-Sifuentes, Neal Yancey, John E. Aston*

5:43 Paper 215h: A Multi-Scale Framework for Simulation of the Impact of Feedstock Variability on Fast Pyrolysis Products — ***James E. Parks***, *Daniel Carpenter, Liqiang LU, William Rogers, M. Brennan Pecha, Gavin Wiggins, Peter N. Ciesielski, Meagan Crowley, Kristiina Iisa, Matthew Wiatrowski, Yupeng Xu, Mehrdad Shahnam, Jordan Klinger, Damon Hartley, Huamin Wang, Erin Webb*

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(216) Green Chemistry and Engineering-I

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-226A

Lindsay Soh, Chair
Wenqin Li, Co-Chair
Clayton Jeffryes, Co-Chair

Sponsored by: Sustainability Science and Engineering

3:30 Paper 216a: Bioinspired, Non-Enzymatic, 'Green' Synthesis of Size Tunable CdS Quantum Dots — *Nur Ozdemir, Joseph Cline, Leah Spangler, Steven McIntosh, Christopher Kiely,* ***Mark Snyder***

3:50 Paper 216b: Tunable Parameters of Switchable Hydrophilicity Solvents — ***Lindsay Soh***, *Ryan Berry*

4:10 Paper 216c: Environmental Evaluations of Replacement of Fluorinated Aqueous Fire-Fighting Foams (AFFF) — ***William Barrett***

4:30 Paper 216d: A Toolbox to Support the Development of Safe and Sustainable By Design Chemicals, Materials and Products — ***Dimosthenis Sarigiannis***, *Spyros Karakitsios, Antonis Gypakis*

4:50 Paper 216e: Sustainable Design and Life Cycle Assessment of Plant-Based Heme Protein — ***Rui Shi***, *Luis Huezo, Nicholas Schneider*

5:10 Paper 216f: Computer Aided-Design of Cellulose Process from Cannabis Hemp Residues — ***Josè Convers***, *Jeffrey Leòn Pulido, Brigitte Baptiste*

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(217) Novel Approaches to CO_2 Utilization II

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-226C

Gregory Kline, Chair
Damilola Daramola, Co-Chair
Joseph Stoffa, Co-Chair

Sponsored by: Sustainable Energy

3:30 Paper 217a: Carbon-Negative Soda Ash (CODA) — ***Peter Schulze***, *Somayyeh Ghaffari, Maria F. Gutierrez, Heike Lorenz, Andreas Seidel-Morgenstern*

3:45 Paper 217b: Catalytic Conversion of CO_2 over La_2O_3 and CeO_2 Supported Catalysts — ***Parisa Ebrahimi***, *Anand Kumar, Majeda Khraisheh*

4:00 Paper 217c: Design, Validation, and Assessment of a Novel CO_2-Utilized Formic Acid Production Process: Including Techno-Economic Analysis (TEA) and Life-Cycle Assessment (LCA) — ***Changsoo Kim***, *Heewon Lee, Ung Lee*

4:15 Paper 538e: Heterojunction Engineering of BiOCl for Photocatalytic Conversion of CO_2 into Fuels — ***Deeksha Pandey***, *Raju Kumar Gupta*

4:30 Paper 217e: Synthesis of Novel 3DOM-Prevoskites Redox System for CO_2 based Oxidative Ethane Dehydrogenation with Integrated Carbon Capture — ***Sonit Balyan***, *Kyle Vogt-Lowell, Dennis Chacko, Junchen Liu, Fanxing Li, Jianli Hu*

4:45 Paper 217f: Interfacing Electrochemical and Biological Processes Enables Efficient Bioproducts Synthesis from CO_2 — ***Peng Zhang***, *Susie Dai, Joshua Yuan*

5:00 Paper 217g: Step-Wise Rare Earth Elements Recovery and CO_2 Utilization Via pH Swing Carbonation of Alkaline Industrial Waste — ***Seokyoon Moon***, *Hunter Vibbert, Whai Shin Ooi, Aaron Moment, Ah-Hyung Alissa Park*

5:15 Paper 217h: Reactive Water Sorbents for Sorption Enhanced Reverse Water Gas Shift — ***Johannis AZ Pieterse***

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(218) Applications of Data Science in Molecular Sciences II

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-230

Connor Coley, Chair
Johannes Hachmann, Co-Chair
Qing Zhao, Co-Chair

Sponsored by: Applications of Data Science to Molecules and Materials

3:30 Paper 218a: Discovery of O_2-Selective Metal-Organic Frameworks Via Bayesian Optimization — ***Eric Taw***, *Jeffrey B. Neaton*

3:45: Break

4:00 Paper 218c: Cript: A Scalable Polymer Material Data Structure — ***Dylan Walsh***, *Bradley Olsen, Klavs Jensen*

4:15 Paper 218d: Data-Driven Design of Polymer-Protein Hybrid Materials — ***Michael Webb***

4:30 Paper 218e: Applications of Machine-Learned Electron Densities of Nucleic Acids — *Alex Lee, Joshua A. Rackers,* ***William P. Bricker***

4:45 Paper 218f: Using Machine Learning Approaches to Estimate Enzyme Kinetic Parameters — ***Veda Sheersh Boorla***, *Costas D. Maranas*

5:00 Paper 218g: Classifying the Toxicity of Pesticides to Honey Bees Via Support Vector Machines with Random Walk Graph Kernels — *Ping Yang, Adrian Henle, Xiaoli Fern,* ***Cory Simon***

5:15 Paper 218h: Hallucinating Inexpensive, Diverse and Native-like Antibody Binders with Deep Learning — ***Sai Pooja Mahajan***, *Jeffrey Ruffolo, Rahel Frick, Jeffrey J. Gray*

5:30 Paper 218i: Identifying Novel Fentanyl Analogs from Mass Spectral Measurements — ***Arun S. Moorthy***, *Anthony J. Kearsley, William E. Wallace III*

5:45 Paper 218j: Developing a Defeatured Atom-Additive Model to Predict Single Component Partition Coefficients with FT-ICR MS Data — ***David Kenney***, *Heather LeClerc, Randy Paffenroth, Michael T. Timko, Andrew R Teixeira*

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(219) Chemical Engineering Principles Advancing Medicine II

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-126C

Joshua Ramsey, Chair
Varghese Kurian, Co-Chair

Sponsored by: Chemical Engineers in Medicine

3:30 Paper 153e: Genetically Stable CRISPR-Based Kill Switches for Engineered Microbes — *Austin Rottinghaus, Aura Ferreiro, Gautam Dantas,* ***Tae Seok Moon***

3:51 Paper 219b: Virus Encapsulation in Polypeptide Complex Coacervates for Vaccine Formulations — ***Caryn Heldt***, *Pratik Joshi, Claire Decker, Xianci Zeng, Arvind Sathyavageeswaran, Sarah Perry*

4:12 Paper 219c: Association and Adsorption of Mucins to the Air Interface in Human Airway Mucus — ***Scott Danielsen, PhD***, *Richard C. Boucher, Michael Rubinstein*

4:33 Paper 219d: Computational Fluid Dynamics to Understand Ureteroscopy Irrigation — ***David G. Foster***

4:54 Paper 219e: Validation of Stroke Prediction in Patients with Carotid Artery Disease Using CFD — ***David G. Foster***, *Lauren Redus*

5:15 Paper 219f: A Computational Predictive Framework Towards Individualized Risk Assessment of Kidney Transplantation Failure. — ***Symeon Savvopoulos***, *Andreas I. Reppas, Wilfried Gwinner, Irina Scheffner, Haralampos Hatzikirou*

5:36 Paper 219g: Monte Carlo Simulations of Spherocylinders Interacting with Site-Dependent Square Well Potentials — ***Kiranmai Yellam***, *Prateek Jha*

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(220) Plasma Catalysis

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-227A

Maria Carreon, Chair
Ryan Hartman, Co-Chair

Sponsored by: Material Interfaces as Energy Solutions

3:30: Introductory Remarks

3:33: Break

3:54 Paper 220b: Chemical Looping Ammonia Synthesis: Thermal, Microwave, and Plasma Approaches — ***Sean Brown***, *Brandon Robinson, Jianli Hu*

4:15 Paper 220c: Pathways for NH_3 Formation from N, H, and N_2(v) in Plasma Catalysis — ***Brian Bayer***, *Peter Bruggeman, Aditya Bhan*

4:36 Paper 220d: Accessing Meta-Stable States through Plasma Catalysis — ***Casey O'Brien***, *Garam Lee, David Go*

4:57 Paper 220e: Methane Dehydroaromatization over Mo/H-ZSM-5 Under Non-Thermal Plasma Stimulation — ***Gerardo Rivera-Castro***, *Jason Hicks*

5:18 Paper 220f: Recombination after the Plasma and Product Distribution — *Colin Page,* ***Elijah Thimsen***

5:39 Paper 220g: A Novel Pulsed-Plasma Catalytic Reactor for Dry Reforming of Methane — ***Michael Mullins***, *Ben Caithamer*

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(221) 3D Printing of Composites

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-221B

Kenan Song, Chair
Mohammad Azad, Co-Chair

Sponsored by: 3D Printing

3:30 Paper 221a: High-Resolution 3D Printing of Piezoelectric Structures Using Micro-CLIP — *Siying Liu, Wenbo Wang, Luyang Liu,* ***Xiangfan Chen***

3:50 Paper 221b: Enabling Off-Earth Construction and Isru through 3D Printing of Dense Regolith Suspensions — ***Alexandra Marnot***, *Blair Brettmann*

4:10 Paper 221c: 3D Printing of Thermoset/Mxene Composites with Layered Hierarchies — ***Sayli Jambhulkar***, *Kenan Song*

4:30 Paper 221d: Fabrication and Evaluation of Highly Filled Polymer-Based Multi-Layer Filament for Fused Deposition Modeling (FDM) — ***Juhyeong Lee***, *Jay Park*

4:50 Paper 221e: Direct-Write Printing of Metal-Carbon Nanotube Composites for High-Performance Electronics — ***Crystal Owens***, *A John Hart*

5:10 Paper 221g: Three-dimensional photochemical printing of thermally activated polymer foams — ***S. Eileen Seo***, *Younghoon Kwon, Megan T. Valentine, Craig J. Hawker*

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(222) Industrial Internet of Things (IIoT), Smart and Soft Sensors in Process Manufacturing and Beyond

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-221A

Zhenyu Wang, Chair
Helen Lou, Co-Chair
Xiaonan Wang, Co-Chair

Sponsored by: Next-Gen Manufacturing

3:30 Paper 222a: Keynote Talk-Industrial Internet of Things at Dow Inc. — ***Mary Beth Seasholtz***

3:55: Break

4:12 Paper 222c: Sensor Placement for Process Networks Based on the Sensitivity Analysis — ***Siyu Liu***, *Jinfeng Liu, Xunyuan Yin*

4:29 Paper 222d: Development of AI Algorithms for Corrosion Prediction in Midstream Industry — ***Helen Lou***, *Jian Fang, Sidney Lin*

4:46 Paper 222f: Physics-Informed Surrogate Models for Manufacturing Applications — ***Utsav Awasthi***, *George M. Bollas*

5:03 Paper 222g: Enhancing Operator's Trust in AI-Based Process Monitoring Technologies: Providing Explanations for Multi-Mode Processes — ***Abhijit Bhakte, Piyush Kumar Kumawat, Rajagopalan Srinivasan***

5:20 Paper 222h: Evaluating Controllers for Next-Generation Manufacturing — ***Fnu Akkarakaran Francis Leonard***, *Keshav Kasturi Rangan, Ilham Azali Assoumani, Jacob Noll, Carley Fields, Nazir Jairazbhoy, Emmanuel Dannug, James Redman, Helen Durand, K.Y. Simon Ng*

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(223) Next-Gen Sensors

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-231A

Jeffrey Halpern, Chair
Chelsea Monty-Bromer, Co-Chair

Sponsored by: Sensors for Sustainability

3:30 Paper 223a: Invited Talk: Fabricating Ordered Nanoparticle Arrays for Biosensing Platforms Via Scanning Electrochemical Cell Microscopy — *Md Maksudur Rahman, Jeffrey Halpern,* ***Caleb Hill***

3:55 Paper 223b: Anomaly Detection Algorithms to Utilize Non-Injective Gas Sensor Arrays — ***Paul Morris***, *Cory Simon*

4:10 Paper 223c: A Novel Sensing Technology for Online Detecting Reaction State and Fluid Mixing Using Electrical Resistance Tomography — *Braden Hoff,* ***Weiguo Xie***

4:25 Paper 223d: Ag-CNT-Silicone Based Piezoresistive Tactile Sensor with< 200 Mm Spatial Resolution for Large Area Artificial 3D-Curved Skin Deployment and Posture Stability Applications — ***Muhammad Haider***

4:40 Paper 223e: Vapor Phase Eta-6 Surface Functionalization of Hexagonal Boron Nitride Films — *Vikas Berry,* ***Kartikey Sharma***, *Songwei Che, Sanjay Behura*

4:55 Paper 223f: Investigation of Surface-Bound ELP As a Thermoresponsive Polymer Film — ***Stanley Feeney***, *Zahra Panahi, Eva Rose M. Balog, Jeffrey Halpern*

5:10 Paper 223g: Responsive Complex Emulsions: All-Liquid Sensors for Biomolecules and Environmental Pollutants — ***Suchol Savagatrup***

5:25 Paper 223h: On-Chip Infrared Spectroscopy with Near-Field Detection — ***Sean McSherry***, *Andrej Lenert*

5:40 Paper 223i: Possibility of Energy Harvesting Wireless Sensors Using Magnetic Phase Transition — ***Yasuki Kansha***, *Hikaru Kiyomoto, Yuka Sakai, Yuki Sato*

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(224) Chemical Engineering Applications in the Nuclear Industry

Monday, Nov 14, 4:15 PM
Phoenix Convention Center, N-224AB

Courtney Bottenus, Chair
Philip Schonewill, Co-Chair

Sponsored by: Nuclear Engineering Division

4:15 Paper 224a: Process Challenges and Changes in the Sludge Batch 10 Flowsheet at the Defense Waste Processing Facility — ***Wesley Woodham***, *Anthony Howe, Matthew Siegfried*

4:32 Paper 224b: Development and Implementation of the Next Generation Solvent Flowsheet at the Salt Waste Processing Facility — ***Wesley H. Woodham***, *Thomas Peters, Seth Hunter*

4:49 Paper 224c: Speciation of Aluminum Phases at the Hanford Site — *Amy Westesen,* ***Reid Peterson***

5:06 Paper 224d: Review of Fire Safety Analyses Conducted at the Savannah River Site — ***James Laurinat***

5:23 Paper 224e: Multi-Scale Comparison of Supernatant Tank Waste Hydraulic Performance — ***Philip Schonewill***, *Phillip A. Gauglitz, Richard Daniel, Carolyn A. Burns*

5:40 Paper 224f: Techno-Economic Assessment of Nuclear Production of Hydrogen for Refining Applications in Saudi Arabia — ***Yousef Alshammari***

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(225) MAC Eminent Engineers Awards Poster Session

Monday, Nov 14, 11:00 AM
Phoenix Convention Center, North Hall E

Nabila Shamim, Chair

Sponsored by: Minority Affairs Committee (MAC)

Poster : Water Orientation and Dynamics in Cavitand Pockets — ***Busayo Alagbe***, *Bruce C. Gibb, Henry Ashbaugh*

Poster : Computational Studies of the Order-Disorder Transition in Block Copolymer Topological Blends — ***Rahul Kumar***, *Amy Goodson, Oluwafemi Alli, Clayton Chamness, Isabella Miserocchi, Julie Albert, Henry Ashbaugh*

Poster : Non-Isothermal Crystallization Kinetics of Poly (ε-caprolactone) (PCL) and MgO Incorporated PCL Nanofibers — ***Daisaku Gicheha***, *Nabila Shamim*

Poster : Bench-Scale Testing of Electrochemical Recovery of Phosphorus from Post-Digester Municipal Wastewater Driven By Magnesium Salt - MAC Poster Session — ***Lawrence Ajayi***, *Sana Heydarian, Jason Trembly, Damilola Daramola*

Poster : Evaluating Transport Factors to Understand Electrochemical Nutrient Removal and Recovery from Synthetic Animal Wastewater- MAC Poster Session — ***Sana Heydarian***, *Francesca Carney, Damilola Daramola*

Poster : Transfer Learning Framework for Catalysis — ***Gbolade Kayode***

Poster : Conceptual Design of Nano-Straws in Spherical Porous Particles for Improved Adsorption Capacity for Carbon Capture — ***Oluwole Ajumobi***

Poster : Evaluating the Role of Carbon Microspheres in an Aqueous Lubricant - the Stribeck Curve Analysis — ***Samuel Solomon***, *Noshir Pesika*

Poster : Bioconversion of Plastic Wastes into Value-Added Products Using Thermal Oxo-Degradation — ***Efrain Rodriguez-Ocasio***, *Mark Blenner, Laura R. Jarboe*

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(226) Topical Plenary: Venture Hour at the AIChE Annual

Monday, Nov 14, 4:45 PM
Phoenix Convention Center, W-103B

Henry Uyeme, Chair

Sponsored by: Entrepreneurship in Chemical Engineering

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(227) MAC Eminent Engineers Awards Ceremony Breakfast

Monday, Nov 14, 9:00 AM
Phoenix Convention Center, N-231B

Bryan Deschamps, Chair

Sponsored by: Minority Affairs Committee (MAC)

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(228) Catalyst Design, Synthesis, and Characterization IV: Zeolites

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-127C

George Tsilomelekis, Chair
Andrew Adamczyk, Co-Chair
Saurabh Bhandari, Co-Chair

Sponsored by: Catalysis

8:00 Paper 228a: Designing Zeolite Catalysts with Enhanced Diffusion Properties — ***Kumari Shilpa***, *Thuy T. Le, Heng Dai, Jeffrey Rimer*

8:18: Break

8:36 Paper 228c: Effect of Pd Speciation on CH_4 Oxidation and Passive NOx Adsorption/Desorption Performance over Zeolite-Based Catalysts — ***Tala Mon***, *Chih-Han Liu, Junjie Chen, Eleni Kyriakidou*

8:54 Paper 228d: Quantifying Active Catalytic Sites in Lewis Acidic Zeolite Sn-Beta — ***Leah Ford***, *Nicholas Brunelli*

9:12 Paper 228e: Elucidating the Impact of Organic Structure Directing Agent Isomer Ratios on the Aluminum Distribution in SSZ-39 — *Charles Umhey IV, Jiawei Guo, Zheng Cui, Ambarish Kulkarni, Daniel Shantz,* ***Jean-Sabin McEwen***

9:30 Paper 228f: Spatial Proximity Influence on Adsorbate Thermodynamics over Zeolite Surfaces — ***Ajibola Lawal***, *Omar Abdelrahman*

9:48 Paper 228g: Characterizing Acid Sites of Phosphorus-Containing Zeosils — *Gaurav Kumar, Limin Ren, Yutong Pang, Xinyu Li,* ***Han Chen***, *Jason Gulbinski, Paul Dauenhauer, Michael Tsapatsis, Omar Abdelrahman*

10:06 Paper 228h: Evolution of Framework Al Arrangements in CHA Zeolites during Crystallization in the Presence of Organic and Inorganic Structure-Directing Agents — ***Songhyun Lee***, *Yujia Wang, Claire Nimlos, Elijah R. Kipp, William Schneider, Marcella Lusardi, Vivek Vattipalli, Subramanian Prasad, Ahmad Moini, Rajamani Gounder*

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(229) Catalytic Upcycling of Waste Plastics I: Focus on Commodity Plastic Waste

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-128A

Wan-Ting Chen, Chair
Deeksha Jain, Co-Chair
Konstantinos Goulas, Co-Chair

Sponsored by: Catalysis

8:00 Paper 229a: Valorization of Polyolefin Waste Streams By Lubricant Production — ***Meltem Urgun-Demirtas***, *Massimiliano Delferro, Aaron Sadow, Pahola Thathiana Benavides, Ulises Gracida Alvarez*

8:18 Paper 229b: Single Step Catalytic Advanced Conversion of Plastic Waste with 85% Olefin Yield — ***Kevin Van Geem***, *Andreas Eschenbacher, Robin John Varghese, G. D. Stefanidis, Evangelos Delikonstantis*

8:36 Paper 229c: Selective Hydrogenolysis of Polyolefin Waste to Liquid Hydrocarbons over Bifunctional Ru/Acid Catalysts — ***Julie E. Rorrer****, Amani Ebrahim, Ydna M. Questell-Santiago, Clara Troyano-Valls, Arun Asundi, Simon Bare, Gregg T. Beckham, Yuriy Roman*

8:54 Paper 229d: Catalytic Co-Pyrolysis of Ldpe and PET with HZSM-5, H-Beta, and HY: Experiments and Kinetic Modeling — ***Hilal Ezgi Toraman****, J.V. Jayarama Krishna, Sean Okonsky*

9:12 Paper 229e: Catalyst Design Strategy for Polypropylene Upcycling to Lubricants Via Hydrogenolysis — ***Pavel Kots****, Brandon Vance, Dionisios Vlachos*

9:30 Paper 229f: Catalytic Co-Pyrolysis of Polyurethane Waste and Lignocellulosic Biomass with Two-Dimensional Zeolites — ***Thossaporn Onsree****, Kanan Shikhaliyev, Andrew Jaeschke, Jochen Lauterbach, Nakorn Tippayawong*

9:48 Paper 229g: Selective Dechlorination Mechanisms with Molecular Catalysts – a Step Towards Polyvinylchloride Upcycling — *Selin Bac, Megan Fieser,* ***Shaama Mallikarjun Sharada***

(230) Fundamentals of Catalysis and Surface Science IV: Model catalytic surfaces

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-128B

Alexander Mironenko, Chair
Adam Nielander, Co-Chair

Sponsored by: Catalysis

8:00 Paper 230a: Tuning Selective Interactions with Free-Atom-like States on Single Atom Alloys — ***Taylor Spivey****, Adam Holewinski*

8:20 Paper 230b: Tuning Reactivity in Trimetallic Dual Atom Alloys: Molecular-like States and Ensemble Effects — ***Shengjie Zhang****, Matthew Montemore*

8:40 Paper 230c: Understanding the Selectivity of Single Atom Alloys in Complex Reaction Pathways: Examining Electrochemical Nitrate Reduction Reaction through Ab-Initio Calculations. — ***Srishti Gupta****, Matthew Shaffer, Adam Chismar, Daniel J. Rivera, Christopher L. Muhich*

9:00 Paper 230d: Identification of the Local Configurations and Reaction Mechanism of Single-Atom Ir/TiO_2 Catalysts for CO Oxidation — ***Liping Liu****, Coogan Thompson, Ayman M. Karim, Hongliang Xin*

9:20 Paper 230e: Mechanistic Insights into CO Oxidation over Pt_1/TiO_2: Site-Sensitivity and Dynamic Character of Single Atoms — ***Selin Bac****, Nicholas Humphrey, Shaama Mallikarjun Sharada*

9:40: Break

10:00 Paper 230g: Modeling Distribution Tendencies of Noble Metals on Fe(100) — ***Isaac Onyango****, Gregory Collinge, Jean-Sabin McEwen, Yong Wang*

(231) In Honor of the 2020 R.H. Wilhelm Award Winner I (Invited Talks)

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-127A

Marc Porosoff, Chair
Daniel Esposito, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

8:00: Welcoming Remarks

8:03 Paper 231a: Electron-Driven Nitrogen Transformations: Decarbonizing Ammonia Using Plasma Catalysis and Electrochemical Reduction of Nitrate in Wastewaters — ***Lea Winter***

8:24 Paper 231b: General Descriptors for Steering CO_2-Assisted Selective C—H/C—C Bond Scission in Ethane — ***Zhenhua Xie****, Jingguang G. Chen*

8:45 Paper 231c: Enhancing the Tandem Reactions of CO_2-Assisted Ethane Dehydrogenation and Aromatization — ***Elaine Gomez****, Xiaowa Nie, Ji Hoon Lee, Zhenhua Xie, Jingguang G. Chen*

9:06 Paper 231d: The Power of Circularity – Challenges and Opportunities — ***MyatNoeZin Myint***

9:27 Paper 231e: Novel Catalytic Approach Towards C4 Olefins and Gasoline Octane in Fluid Catalytic Cracking — ***Yuying Shu****, Edwin Yik, Mike Ziebarth, Bani Cipriano, Chad Cavan, Wu-Cheng Cheng*

9:48 Paper 231f: Development of Tandem Catalysts for Carbon Dioxide Hydrogenation to Olefins — ***Marc Porosoff***

10:09 Paper 231g: Everything I Need to Know about Catalysis I Learned from Dr. Chen — ***William Lonergan***

(232) Pioneers of Catalysis and Reaction Engineering (Invited Talks)

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-127B

Bihter Padak, Chair
Sheima Khatib, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

8:00 Paper 232a: Cation and Nanoparticle Interconversion in Metal-Exchanged Zeolites — ***Christopher Paolucci***

8:30 Paper 232b: Catalyst Development for Sustainable Technologies: From Fundamentals to Commercialization — ***Deeksha Jain***

9:00 Paper 232c: Resonance-Enhanced Hydrocarbon Oxidation Via Programmable Catalysis — ***Omar Abdelrahman***

9:30 Paper 232d: Creating Value from CO_2: The Development of Sorption-Enhanced Catalysts to Promote a Circular Economy — ***Kandis Leslie Gilliard-AbdulAziz***

10:00 Paper 232e: Designing Dual Function Materials for Integrated Carbon Dioxide Capture and Utilisation — ***Melis Duyar***

(233) Recent Advances in Multiscale Methodologies

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-222B

Kayla Sprenger, Chair
Dinesh Sundaravadivelu Devarajan, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

8:00 Paper 233a: Symmetric Molecular Dynamics — ***Andrew White***

8:22 Paper 233b: An Extended-Ensemble Relative Entropy Approach to Sequence-Specific Coarse-Grained Models for Peptide Aggregation — ***Evan Pretti****, M. Scott Shell*

8:38 Paper 233c: Drl Take the Wheel: Employing Deep Reinforcement Learning to Drive Vaccine Models — ***Jonathan Faris****, Daniel Orbidan, Brenden Petersen, Kayla Sprenger*

8:54 Paper 233d: Accelerated Kinetic Monte Carlo (kMC) Simulation and Density Functional Theory (DFT) to Predict Turn-over Frequencies in Heterogeneous Complex Catalytic Reactions — ***Silabrata Pahari****, Chi-Ho Lee, Joseph Kwon*

9:10 Paper 233e: Towards the Elimination of Backmapping in Multiscale Simulations — ***Nicholas Jackson***

9:26 Paper 233f: Implicit Heuristic Model Captures Electrostatic Features of Cell Membrane Environment — ***Rituparna Samanta****, Jeffrey J. Gray*

9:42 Paper 233g: Hamiltonian-Resolution Replica Exchange Improves Flexible Backbone Protein Docking By Mimicking Induced-Fit Pathways — ***Ameya Harmalkar****, Jeffrey J. Gray*

9:58 Paper 233h: Modeling the Influence of Glycosylation on Protein Interaction — *Bradley Harris, Yihan Huang, Zachary Rollins, Karen A. McDonald, Somen Nandi, Priya Shah, Steven George,* ***Roland Faller***

10:14 Paper 233i: Multiscale Molecular Modeling of Flory-Huggins χ-Parameter Calculation and Simulation of Structural Transformation of Photo-Regulated Multicompartment Micelle — ***Jinwon Cho***, *Ji Il Choi, Seung Soon Jang*

(234) Advances in Nonlinear and Surrogate Optimization

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, W-101C

Andrew Allman, Chair
M M Faruque Hasan, Co-Chair

Sponsored by: Systems and Process Operations

8:00 Paper 234a: New Measures for Shaping Trajectories in Dynamic Optimization — ***Joshua Pulsipher***, *Benjamin Davidson, Victor Zavala*

8:18 Paper 234b: An Implicit Function Formulation for Optimization of Discretized Index-1 Differential Algebraic Systems — ***Robert Parker***, *Bethany Nicholson, John Siirola, Carl Laird, Lorenz Biegler*

8:36: Break

8:54 Paper 234d: Learning to Initialize Generalized Benders Decomposition — ***Ilias Mitrai***, *Prodromos Daoutidis*

9:12 Paper 234e: Global Convergence Analysis of Data-Driven Spatial Branch-and-Bound Algorithms — ***Suryateja Ravutla***, *Jianyuan Zhai, Fani Boukouvala*

9:30 Paper 234f: Exploiting Grey-Box Hybrid Models in Constrained Bayesian Optimization Using a Smoothed Sample Average Approximation — ***Congwen Lu***, *Joel Paulson*

9:48 Paper 234g: A Novel Surrogate-Based Derivative-Free Optimization Algorithm — ***Bianca Williams***, *Selen Cremaschi*

10:06 Paper 234h: A Benders Decomposition Framework for the Optimization of Generalized Disjunctive Programming Problems with Ordered Boolean Variables — *David A. Linan,* ***Luis Ricardez-Sandoval***

(235) Advances in Process Control I

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, W-101B

Ravendra Singh, Chair
Daniel Rivera, Co-Chair

Sponsored by: Systems and Process Control

8:00 Paper 235a: Barrier Function-Based Predictive Controllers Compared with Lyapunov-Based Economic Model Predictive Control — ***Helen Durand***, *Aaron Ames, Prithvi Akella*

8:19 Paper 235b: Online Construction of Achievable and Feasible Funnels for Transient Constraints of Model Predictive Controllers — ***San Dinh***, *Fernando V. Lima*

8:38 Paper 235c: Dynamic Real Time Optimization with Embedded Closed-Loop Lyapunov Stabilizing MPC — ***Lloyd MacKinnon***, *Praveen Sundaresan Ramesh, Prashant Mhaskar, Christopher Swartz*

8:57 Paper 235d: Controller Switching to Facilitate the Detection of Multiplicative Cyberattacks on Nonlinear Process Systems — ***Shilpa Narasimhan***, *Nael El-Farra, Matthew Ellis*

9:16 Paper 235e: Generic Semi-Infinite Stochastic Programming Formulation and Algorithm for Control-Lyapunov Function Design — ***Wentao Tang***, *Prodromos Daoutidis*

9:35 Paper 235f: Data-Efficient Globally Optimal Policy-Based Reinforcement Learning Via Gradient-Accelerated Bayesian Optimization — ***Joel Paulson***, *Georgios Makrygiorgos, Ali Mesbah*

9:54 Paper 235g: Computer Vision Aided Process Control: Methods for Enhanced Autonomy and Robustness — ***Joshua Pulsipher***, *Luke Coutinho, Victor Zavala*

10:13 Paper 235h: Towards Multivariable Optimization and Control for a Perfusion Bioreactor System in Tissue Engineering — ***Ioana Nascu***, *Ioan Nascu, Tao Chen, Wenli Du*

(236) Software Tools and Implementations for Process Systems Engineering

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, W-101A

Matthew Stuber, Chair
Victor Zavala, Co-Chair
Fernando V. Lima, Co-Chair

Sponsored by: Computing Systems and Technology Division

8:00 Paper 236a: An Open-Source Python-Based Toolbox for Enabling Fast Process Operability Calculations — ***Victor Alves***, *San Dinh, Fernando V. Lima*

8:18 Paper 236b: Omlt: Optimization and Machine Learning Toolkit — *Francesco Ceccon, Jordan Jalving, Joshua Haddad, Alexander Thebelt,* ***Calvin Tsay***, *Carl Laird, Ruth Misener*

8:36 Paper 236c: GEMS: A Framework for Surrogate Modeling and Optimization with Guaranteed Error Bounds — ***Ashfaq Iftakher***, *Chinmay Aras, Mohammed Sadaf Monjur, M M Faruque Hasan*

8:54 Paper 236d: Energiapy - a Decision-Making and Risk Management Tool for Multi-Scale Modeling and Optimization — ***Rahul Kakodkar***, *Moustafa Ali, Shivam Vedant, Efstratios N. Pistikopoulos*

9:12 Paper 236e: Software and Advanced Solution Methods for Flexibility Analysis — ***Michael Bynum***, *Bashar Ammari, Ignacio Grossmann, Taehun Kim, Carl Laird, Joshua Pulsipher, John Siirola, Stephen Zitney*

9:30 Paper 236f: Pyomo.Doe: An Open-Source Package for Model-Based Design of Experiments in Python — ***Jialu Wang***, *Alexander Dowling*

9:48 Paper 236g: Comando: An Open-Source Python Package for Optimal Design and Operation of Energy Systems — *Marco Langiu, David Yang Shu, Florian Joseph Baader, Dominik Hering, Uwe Bau, André Xhonneux, Dirk Müller, André Bardow,* ***Alexander Mitsos***, *Manuel Dahmen*

10:06 Paper 236h: Recent Developments in EAGO.jl (Easy Advanced Global Optimization in Julia) — ***Robert Gottlieb***, *Matthew Wilhelm, Pengfei Xu, Matthew Stuber*

(237) Free Forum on Engineering Education: First Year and Sophomore Year

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, W-102A

Fernando Mérida Figueróa, Chair
Joseph Chada, Co-Chair

Sponsored by: Undergraduate Education

8:00: Welcoming Remarks

8:02 Paper 237a: Teaching Chemical Engineering with Coffee: Lessons Learned with 1,800 Students per Year — ***William Ristenpart***, *Tonya L. Kuhl*

8:20 Paper 237b: Using an Aeropress Coffee Brewer to Teach Fluid Mechanics — ***Kristen E. Fawole***, *Kristen Fawole, Tonya L. Kuhl, William Ristenpart*

8:38: Break

8:56 Paper 237d: Attracting Sophomores to Careers in Process Control and Automation through a Winter Term Workshop and Targeted Internships — ***Jason Berberich***, *Douglas Coffin, Gary Rudemiller, Patrick Dixon, Keith Hohn*

9:14 Paper 237e: Mastery Learning in the Mass Balances Class — ***Payton Kamer***, *Glenn Lipscomb*

9:32 Paper 237f: Relating "Mass and Energy Balances" Concepts to Everyday Life and Developing Professional Skills — ***Cody Mischel***, ***Betul Bilgin***, *James Pellegrino, Lewis Wedgewood, Vikas Berry*

9:50 Paper 237g: Teaching and Learning Strategy of Aspenone during COVID-19 Pandemic to Chemical Engineering Sophomores — ***Sushobhan Pradhan***, *Sundararajan Madihally*

10:08 Paper 237h: Imperial Chemical Engineering Wiki: The Development, Lessons Learned and Future Growth of Student-Led Wikis in Engineering Education — *Luc Paoli, **Thomas Nok Hin Cheng**, Pierre Walker, David -, Marsha Maraj, Jerry Y. Y. Heng*

(238) In Honor of the 2021 Recipient of the Warren K. Lewis Award - Nicholas Peppas - Part I (Invited Talks)

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, W-105A

Antonios Mikos, Chair
Surya Mallapragada, Co-Chair

Sponsored by: Education

8:00: Introductory Remarks

8:15 Paper 238a: Teaching Better Biomedical Engineering: Sixty Years of Chemical Engineering Contributions That Shaped up Bioengineering — ***Nicholas Peppas***

9:00 Paper 238b: Regenerative Engineering Education and Democratization of Science: The Uconn-M1 Program — ***Cato Laurencin***

9:30 Paper 238c: Sowing the Seeds of Diversity in Engineering Via Mentoring — ***Jennifer Curtis***

10:00 Paper 238d: Perspectives and Suggestions on How to Advance Underrepresented Minority (URM) Faculty at Minority Serving Institutions — ***Carlos Rinaldi-Ramos***

(239) Safety in ChE: How ChE Departments are Satisfying the AIChE Program Criteria

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, W-105B

Donald Visco Jr., Chair
Troy Vogel, Co-Chair
Thomas Spicer III, Co-Chair

Sponsored by: Undergraduate Education

8:00 Paper 239a: How the ChE Education Community Is Satisfying the Institute's Program Criteria Associated with Design, Analysis and Control of Processes: Survey Data from Program Evaluators — ***Donald Visco Jr.**, Thomas Spicer III, Troy Vogel*

8:10 Paper 239b: Integrating Chemical Process Safety into a Chemical Engineering Curriculum — ***Richard Davis**, Weiguo Xie, Michael Rother, Tsutomu Shimotori*

8:30 Paper 239c: Chemical Process Safety: A 3-Credit Course at the University of Florida — ***Mark E. Orazem**, Vincent Tocco Jr., **Helena Hagelin Weaver***

8:50 Paper 239d: A Multi-Dimensional Approach: Applying Process Safety Principles in Several Courses across the Curriculum. — ***Stephanie Loveland**, R. Dennis Vigil, Derrick Rollins Sr.*

9:10 Paper 239e: How We Designed Our Safety Program to Improve Safety Education and Process, and to Satisfy Aiche Program Criteria — ***George Prpich**, Ron Unnerstall*

9:30 Paper 239f: Integrating Process Safety with a Unique Industrial Perspective into the Curriculum at Kansas State University — *Jennifer L. Anthony, **Md Uddin**, **Andrew Duncan**, Christopher Frampton, Chris Aiken*

9:50 Paper 239g: Successful Process Safety Instruction in Two Capstone Design Courses at a Hispanic-Serving Institution — ***Matthew Alexander**, Joseph Amaya*

10:10 Paper 239h: Integrating Process Safety across the Curriculum — ***Tracy Carter***

(240) Allies and Advocates Training

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, N-226B

Shannon Servoss, Chair

Sponsored by: The Role of Intersectionality in Chemical Engineering

(241) Area Plenary: Interfacial Phenomena (Invited Talks)

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-129AB

Marina Tsianou, Chair
Christopher Wirth, Co-Chair

Sponsored by: Interfacial Phenomena

(242) Colloidal Hydrodynamics

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-232A

Sarah Hormozi, Co-Chair
Sara Hashmi, Co-Chair

Sponsored by: Fluid Mechanics

8:00 Paper 242a: Measuring and Modeling Interactions between Orientable Nanoparticles in Flow — *Patrick T. Corona, Jiamin Zhang, L. Gary Leal, **Matthew Helgeson***

8:15 Paper 242b: Toward Understanding the Viscous and Inertial Nonlocal Rheology of Dense Suspensions — ***Sarah Hormozi**, Donald L. Koch*

8:30 Paper 242c: Transient Microstructure, Rheology of Shear-Thickening Colloidal Suspensions By Time-Resolved Flow-SANS and Relation to Nanotribology — *Yu-Fan Lee, **Norman J. Wagner**, Kevin Whitcomb*

8:45 Paper 242d: Effect of Particle Roughness on Shear-Induced Diffusion — ***Han Zhang**, Phong Pham, Bloen Metzger, Dmitry I. Kopelevich, Jason E. Butler*

9:00 Paper 242e: An Anisotropic Clustering Instability Due to Inter-Particle Hydrodynamic and Magnetic Interactions in a Sheared Magnetorheological Fluid Subject to a Magnetic Field — ***V Kumaran***

9:15 Paper 242f: Shear-Driven Ordering and Disordering of 2D Frictional Sphere Suspensions — ***Abhishek Sharma**, Abhinendra Singh, Juan J. de Pablo*

9:30 Paper 242g: Viscoelasticity and Creep Memory of Rough Colloids — ***Lilian Hsiao**, Shravan Pradeep, Yug Saraswat*

9:45 Paper 242h: Axisymmetric Stokes Flow Past a Colloidal Particle — ***Amir Nourhani**, Seyed Amin Nabavizadeh, Mohammad Nabil, Paul E. Lammert*

10:00 Paper 242i: Stokesian Image Systems and Lorentz' Reflection Theorem — ***Nicholas G. Chisholm**, Sarah D. Olson*

10:15 Paper 242j: Dynamics of Elastic Thin Sheets in Stokes Flow: Wrinkling Dynamics in Uniaxial Extensional Flow and Simple Shear Flow — ***Yijiang Yu**, Michael Graham*

(243) Complex Fluids

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-231C

Samanvaya Srivastava, Co-Chair
Sujit Datta, Co-Chair

Sponsored by: Fluid Mechanics

8:00 Paper 243a: Anomalous Rheological Aging of a Model Thermoreversible Colloidal Gel Following a Thermal Quench — ***Khushboo Suman**, Norman J. Wagner*

8:15 Paper 243b: Leveraging Polymer Glass Transition to Access Thermally-Switchable Dense Suspensions — ***Chuqiao Chen**, Michael van der Naald, Abhinendra Singh, Neil Dolinski, Grayson L. Jackson, Heinrich M. Jaeger, Stuart J. Rowan, Juan J. de Pablo*

8:30 Paper 243c: Effect of Colloid Roughness on the Microstructure of Sheared Gels — ***Madhu Venkata Rama Krishna Majji**, James Swan*

8:45 Paper 243d: Multi-Mode Buckling Dynamics of Semiflexible Colloidal Chains — ***Sibani Biswal***

9:00 Paper 243e: Microstructural Dynamics of Rod-like Viruses at High Shear Via Capillary Rheo-SANS — ***Steve Kuei**, Paul F. Salipante, Ryan P. Murphy, Katie Weigandt, Steven D. Hudson*

9:15 Paper 243f: A Constitutive Equation for Dense Emulsions in Unsteady and High Capillary Flows — ***Joseph Peterson**, Vipin Michael, Ioannis Bagkeris*

9:30: Break

9:45 Paper 243h: Probing the Rheology of Block Polymer Liquid Crystals Via Diffusion of Nanometric Tracer Particles — *Connor S. Valentine, **Lynn Walker***

10:00 Paper 243i: Shear-Induced Instability of Blue Phase Liquid Crystals — ***Sepideh Norouzi**, Jose A. Martinez-Gonzalez, Rui Zhang, Monirosadat Sadati*

10:15 Paper 243j: Structural and Rheological Responses of an Entangled Polyethylene Solution to Uniaxial Extensional Flows Via Nonequilibrium Molecular Dynamics Simulations — *Mohammad Hadi Nafar Sefiddashti, Brian J Edwards, **Bamin Khomami***

(244) Computational Studies of Self-Assembly

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-223

Julia Dshemuchadse, Chair
Sumit Sharma, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

8:00 Paper 244a: Dynamic Pathways in Reconfigurable Anisotropic Colloidal Assembly — ***Michael A Bevan***

8:15 Paper 244b: Kinetics of Diffusionless Transitions of Colloidal Truncated Cubes — ***Abhishek Sharma**, Fernando Escobedo*

8:30 Paper 244c: Dynamic Density Functional Theory for Drying Colloidal Suspensions: Comparison of Free Energy Functionals — ***Mayukh Kundu**, Michael Howard*

8:45 Paper 244d: Short-Ranged Forces Enable the Self-Assembly of Binary Nanocrystal Superlattices — ***R. Allen LaCour II**, Emanuele Marino, Timothy C. Moore, Sharon C. Glotzer, Christopher B. Murray*

9:00 Paper 244e: The Role of Iodide in the Solution-Phase Growth of Cu Microplates: A Multi-Scale Theoretical Analysis from First Principles — ***Junseok Kim**, Kristen Fichthorn*

9:15 Paper 244f: Microphase Separation in Diblock Copolymer Material Driven By Solvent Evaporation — ***Ludwig Schneider**, Juhae Park, Juan J. de Pablo*

9:30 Paper 244g: Multilayered Ordered Arrays Self-Assembled from a Mixed Population of Nanoparticles — ***Vikram Jadhao**, Masaki Uchida, Nicholas E. Brunk, Nathasha Hewagma, Trevor Douglas*

9:45 Paper 244h: Simulation Study of Stratum Corneum Lipid Self-Assembly — ***Parashara Shamaprasad**, Christopher Iacovella, Annette Bunge, Clare McCabe*

10:00 Paper 244i: Deciphering the Molecular Features Stabilizing Peptide Bilayer Membrane — ***M. Hamsa Priya***

(245) Symposium on Thermophysical Properties for Industry: Experiments and Models

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-222C

Thomas Knotts IV, Chair
Antonia Statt, Co-Chair
Nav Nidhi Rajput, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

8:00 Paper 245a: Polyolefin Property Estimation using Process Modeling and Machine Learning in Industry — ***Niket Sharma***

8:30 Paper 245b: Going Beyond Accurate Models - What Comes Next in Machine Learning — ***Andrew White***

9:00 Paper 245c: To the Determination of Thermodynamic Properties of g^3 "C_3F_7cn - CO_2 - O_2" Insulating Gas for Electrical Circuit Breaker — ***Driss EL Kinaoui***

9:15 Paper 245d: Modeling of Ultrasonic Polymer Degradation Using Continuous Kinetics — ***David Kruppa**, Jana Zimmermann, Michael Fischlschweiger, Sabine Enders*

9:30 Paper 245e: Predicting Gas Solubility in Semi-Crystalline, Branched Polymers Using Lattice-Cluster-Theory — ***Simon Leube**, Michael Fischlschweiger, Sabine Enders*

9:45: Break

10:00 Paper 245g: A Thermodynamic, Technical, and Economic Evaluation of Hydrogen Blending in Natural Gas Pipelines — ***Ismail Alkhatib**, Ahmed Al Hajaj, Ali Almansoori, Lourdes Vega*

10:15 Paper 245h: Physics-Informed Deep Learning for Prediction of Thermophysical Properties: The Parachor Method for Surface Tension — ***Thomas Knotts IV**, John Hedengren, Mohammad R. Babaei*

(246) Thermodynamic and Transport Properties Under Pressure

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-232C

Erdogan Kiran, Chair
Steven Saunders, Co-Chair

Sponsored by: High Pressure

8:00 Paper 246a: Glass Transition Behavior of Poly(methyl methacrylate) in Compressed Carbon Dioxide Revisited — ***Joseph Sarver**, Grant Van Horn, **Erdogan Kiran***

8:20 Paper 246b: Molecular Interactions in Mixtures of High Molecular Mass Alkanes and Alcohols in the Presence and Absence of Supercritical Carbon Dioxide — ***Cara Schwarz**, Susanna H. du Plessis, Chris F.O. Momoh, Izak A. Cronje, Susan P. Nortje*

8:40 Paper 246c: Effects of Copolymer Composition and Polymer Crystallinity in Thermal Transitions in Carbon Dioxide and Foaming Outcomes of Ethylene Copolymers — ***Joseph Sarver**, Grant Van Horn, Jake Adams, Dokyung Rhee, **Erdogan Kiran***

9:00 Paper 246d: Transport Properties of Ionic Liquids with Compressed Polar Gases — *Karim Al-Barghouti, Rajkumar Kore, **Aaron Scurto***

9:20 Paper 246e: Measurements of the Thermal Conductivity of Dodecane- N_2 Mixtures at Temperatures up to 700 K and Pressures up to 70 Mpa — ***Aaron J. Rowane**, Richard A. Perkins*

9:40 Paper 246f: Fractionation of Guayule Resin Using Supercritical CO_2 — ***Mostafa Dehghanizadeh**, Catherine Brewer*

10:00 Paper 246g: Density and Viscosity of Lubricant Base Oils Modified with Polymeric Additives and Their Correlations — ***Katrina Avery**, **Erdogan Kiran**, John C. Hassler, Mark Devlin*

(247) Tutorial Session on Electrochemical Methods, Systems and Applications (Invited Talks)

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-232B

Matthew Gebbie, Chair
Ariel Furst, Co-Chair
Abdoulaye Djire, Co-Chair
Elizabeth Corson, Co-Chair

Sponsored by: Electrochemical Fundamentals

8:00 Paper 247a: Modeling Porous Electrodes in Fuel Cells and Similar Devices: A Tutorial — ***Adam Weber***

8:35 Paper 247b: Insights into Battery Operation and Degradation through X-Ray Scattering — ***Michael Toney***

9:10 Paper 247c: Rigorous Kinetic Analysis of Electrocatalytic Reactions — ***Karthish Manthiram***

(248) Fundamentals of Environmental Kinetics and Reaction Engineering

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-225A

Rajib Mukherjee, Chair
Matthew Alexander, Co-Chair
Panagiotis Smirniotis, Co-Chair

Sponsored by: Fundamentals

8:00 Paper 248a: Natural and Metal-Impregnated Clays Catalyze the Pyrolytic Treatment of Crude-Oil Contaminated Soils — ***Priscilla Dias da Silva**, Sara Denison, Caroline Koester, Pedro J. J. Alvarez, Kyriacos Zygourakis*

8:25 Paper 248b: Abiotic Degradation of Chlorinated Solvents with Reactive Iron Minerals from Redox Transition Zones — *Xin Yin, Han Hua, James Dyer, Richard Landis, Donna Fennell,* ***Lisa Axe***

8:50 Paper 248c: Chlorine Dioxide Decay in the Presence of Lead Minerals Found in Drinking Water Distribution Systems — ***Christian Lastoskie***

9:15: Break

9:40 Paper 248e: Design of Porous Hybrid Composites with Dual-Adsorption Capacity for Carbon Capture — ***Vijay T. John****, Oluwole Ajumobi, Azeem Farinmade, Julia A. Valla*

10:05 Paper 248f: On-Demand Photocatalyzed Flow Production of Hydrogen Peroxide from Immobilized Anthraquinones — *Hunter Vibbert, Christoph Bendel, Mengqi Shen, Ah-Hyung Alissa Park,* ***Aaron Moment***

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(249) Water Reuse and Recycling

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-225B

Kirti Yenkie, Chair
Toufiq Reza, Co-Chair
Deepak Sharma, Co-Chair

Sponsored by: Water

8:00 Paper 249a: Optimization of a Wastewater Cotreatment Process for Blowdown and Produced Waters with Economic and Sustainability Analyses — ***Hunter Barber****, Victor Alves, Fernando V. Lima*

8:25 Paper 249b: Hydrothermal Gasification of Concentrated Blackwater to Produce Energy and Low-Tier Water — ***Sean Thompson****, Nathaniel Michael, Andrew Wagner, Alex D. Paulsen*

8:50 Paper 249c: Response Surface Optimization for the Development of a Compact, Rapid, and Zero Liquid Discharge Wastewater Treatment System — ***Ramalingam Subramaniam****,* ***Alicia Viera****, Ian Ivey, Jess Fike*

9:15 Paper 249d: Advanced Wastewater Treatment and Management for Water Circularity, Reuse and Recycling — ***Tapas K. Das****, Murilo Innocentini*

9:40 Paper 249e: Treating Hydraulic Fracturing Produced Water By Electrocoagulation — *Mahmood Jebur, Yuhe Cao, Mahdi Malmali, Xianghong Qian,* ***Ranil Wickramasinghe***

10:05 Paper 249f: Impacts of Invasive Species Resulting from Canals — ***Robert Peters****, Tapas Das*

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(250) Advances in Biocatalysts and Biocatalytic Processes

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-125A

Phanourios Tamamis, Chair
Jerome Fox, Co-Chair

Sponsored by: Bioengineering

8:00 Paper 250a: Engineering a Cell-Free System- Enzyme Fusion Scaffold for Biofuel Production — ***Matthew Wong****, Georges Belfort, Mattheos Koffas*

8:18: Break

8:36 Paper 250c: Reductive Enzyme Cascades for Valorization of PET Deconstruction Products Guided By the Specificity of Carboxylic Acid Reductases — ***Madan Gopal****, Roman Dickey, Neil Butler, Michael Talley, Mary Watson, Wilfred Chen, Aditya Kunjapur*

8:54 Paper 250d: Computational Design of Phosphotriesterase for Organophosphate Hydrolysis — ***Jacob Kronenberg****, Maria Kulapurathazhe, Jason Chen, Ashwitha Lakshmi, Stanley Chu, Jin Kim Montclare*

9:12 Paper 250e: The Use of β-Galactosidase to Produce N-Acetyllactosamine As a High Value Molecule Directly from Dairy Whey. — ***Sandra Kentish****, Masih Karimi Alavijeh, Anne Meyer, Sally Gras*

9:30 Paper 250f: Biosynthesis of Triacsin Featuring an *N*-Hydroxytriazene Pharmacophore — ***Antonio Del Rio Flores****, Wenjun Zhang*

9:48 Paper 250g: Bioconversion of CO2 to Value-Added Chemicals — ***Pamela Peralta-Yahya***

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(251) Biomolecular Engineering and the Immune System

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-126A

Xue Sherry Gao, Chair
Whitney Stoppel, Co-Chair
Ashish Kulkarni, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

8:00 Paper 251a: Engineering Dually Adjuvanted Sars-CoV2 mRNA Vaccines — ***Allen Jiang****, Bowen Li, Idris Raji, Caroline Atyeo, Theresa M. Raimondo, Akiva Gordon, Luke Rhym, Galit Alter, Robert Langer, Daniel G. Anderson*

8:18 Paper 251b: Optimizing Combinations of Immune Inhibitors and Agonists to Generate Tolerogenic Antigen Presenting Cells — ***Peter Deak****, Jeremiah Kim, Matthew Rosenberger, Aaron Esser-Kahn*

8:36 Paper 251c: Engineered Multispecific Antibodies to Interrogate and Manipulate Immune Checkpoint Protein Trafficking — *Seth Ludwig,* ***Jamie Spangler***

8:54 Paper 251d: Phospho-Proteomic Analysis of CAR-T Cell Signaling Following Activation By Antigen-Presenting Cancer Cells — ***Melanie MacMullan****, Zachary Dunn, Yun Qu, Xianhui Chen, Pin Wang, Nicholas Graham*

9:12 Paper 251e: Targeting IL-10 to Atherosclerotic Plaques Reduces Vascular Inflammation — *Jeffrey A. Hubbell, Yun Fang,* ***Lisa Volpatti***

9:30 Paper 251f: Apoptotic Bio-Inspired Materials for Targeting and Engineering Macrophage Function — ***Kidochukwu Atube****, Candice Cheung, Michael Gower*

9:48 Paper 251g: Invited Talk: Placeholder for the Invited Talk in Biomolecular Engineering and the Immune System Session — ***Whitney Stoppel****, Xue Sherry Gao, Ashish Kulkarni*

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(252) Cell and Tissue Engineering: Engineering in Aging and Aging Associated Diseases

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-126B

Laurel Hind, Chair
Panagiotis Mistriotis, Co-Chair
Whitney Stoppel, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

8:00 Paper 252a: Organotypic Whole Hemisphere Brain Slice Models to Study the Effects of Age and Oxygen-Glucose-Deprivation on the Extracellular Properties of Cortical and Striatal Tissue — ***Jeremy Filteau****, Elizabeth Nance*

8:18 Paper 252b: Defining Functional Subtypes of Senescence at Single-Cell Resolution — ***Pratik Kamat****, Yukang Li, Bart Starich, Aaron Winston, Anshika Agrawal, Jeremy Walston, Denis Wirtz, Jude Phillip*

8:36 Paper 252c: Age-Dependent Stiffening of the Extracellular Matrix Increases the Rate of Cellular Senescence and Cancer Metastasis — ***Bartholomew Starich****, Joanne Baek, Derin Tanrioven, Pratik Kamat, Jude Phillip, Denis Wirtz*

8:54 Paper 252d: Metabolic Rewiring of Aged Myoblasts and Restores Regenerative Potential of Progeric Skeletal Muscle — ***Nika Rajabian****, Izuagie Ikhapoh, Shahryar Shahini, Ramkumar Thiyagarajan, Aref Shahini, Joseph Kulczyk, Susan Udin, Aimee Stablewski, Kenneth Seldeen, Bruce Troen, Kirkwood Personius, Stelios Andreadis*

9:12 Paper 252e: A Microfluidic Approach for the Isolation of a Highly Migratory Presenescent Stem Cell Subpopulation — ***Farshad Amiri****, Farnaz Hemmati, Panagiotis Mistriotis*

9:30 Paper 252f: Vitamin K2 Modulates Mitochondrial Dysfunction Induced By 6-Hydroxydopamine in SH-SY5Y Cells Via Mitochondrial Quality Control Loop — ***Hengfang Tang Sr.****, Zhiming Zheng*

9:48 Paper 252g: Invited Talk: Placeholder for Invited Talk for the Cell and Tissue Engineering: Engineering in Aging and Aging Associated Diseases Session — ***Whitney Stoppel***, *Laurel Hind, Panagiotis Mistriotis*

(253) Food, Pharmaceutical & Bioengineering Faculty Candidates Session I

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-125B

Thomas J. Mansell, Chair
Adam Melvin, Co-Chair
Ryan Summers, Co-Chair
Mark Blenner, Co-Chair
Whitney Stoppel, Co-Chair
Maobing Tu, Co-Chair

Sponsored by: Food, Pharmaceutical & Bioengineering Division

8:00 Paper 253a: Multi-Scale Modeling of a CHO Production Process Using Integrated Machine Learning Models and Genome-Scale Metabolic Models — ***Saratram Gopalakrishnan***, *Jasmine Tat, Miguel Angel Valderrama-Gomez, Fabrice Schlegel, Pablo A. Rolandi, William Johnson, Cleo Kontoravdi, Nathan Lewis*

8:18 Paper 253b: Mutational Correlation Functions Reveal Patterns of Homologous Recombination across the Bacterial Pangenome — ***Asher Preska Steinberg***, *Mingzhi Lin, Edo Kussell*

8:36 Paper 253c: Constraints on Information Flow in Metabolic Networks — ***Christian Euler***, *Radhakrishnan Mahadevan*

8:54 Paper 253d: Rapid Discovery of Ribosomal Natural Products Using Synthetic Biology Approaches — ***Hengqian Ren***, *Huimin Zhao*

9:12 Paper 253e: A High-Throughput Genome Engineering Approach for Systematic Discovery of Melanin Synthesis Regulators — ***Vivek Bajpai, MD, PhD***, *Tomek Swigut, Joanna Wysocka*

9:30 Paper 253f: Establishing the Biogenesis Process for a Bacterial Organelle — ***Carolyn E. Mills***, *Nolan W. Kennedy, Andre Archer, Svetlana P. Ikonomova, Charlotte Abrahamson, Sasha Shirman, Niall Mangan, Danielle Tullman-Ercek*

9:48 Paper 253g: The Histone H1-like Protein Algp Facilitates Even Spacing of Polyphosphate Granules in *Pseudomonas Aeruginosa* — ***Ravi Chawla***, *Steven Klupt, Vadim Patsalo, Jamie Williamson, Lisa Racki*

10:06 Paper 253h: Dewdrops on the Genome: Regulation of Cell-Identity By Biomolecular Phase Transitions — ***Krishna Shrinivas***

10:24 Paper 253i: Antibody-Lectin Bispecifics for Glyco-Immune Checkpoint Blockade — ***Jessica C. Stark***, *Melissa Gray, Simon Wisnovsky, Nicholas Riley, Carolyn Bertozzi*

(254) Biochemical Conversion Processes in Forest/Plant Biomass Biorefineries

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-228A

Catherine Brewer, Chair

Sponsored by: Forest and Plant Bioproducts Division

8:00 Paper 254a: Chemical Synthesis of Potential Prebiotic Oligosaccharides from Simple Sugars and Lignocellulosic Biomass in Concentrated Acids — ***Meijun Zeng***, *Ning Li, Theresa Astmann, Jee-Hwan Oh, Jan Peter van Pijkeren, Xuejun Pan*

8:15 Paper 254b: Reaction Engineering *in Planta*? Tales of Mass Transfer Limitations and Their Kinetic Consequences at the Mesoscale — ***Nicholas E. Thornburg***, *Ryan M. Ness, Meagan Crowley, Lintao Bu, Michael Pecha, Francois Usseglio Viretta, Vivek Bharadwaj, Yudong Li, Xiaowen Chen, David A. Sievers, Edward Wolfrum, Michael G. Resch, Peter N. Ciesielski*

8:30 Paper 254c: Catalytic Conversion of Bioresource to Graphene-Based Materials — *Théotime Béguerie*, ***Elsa Weiss-Hortala***, *Ange Nzihou*

(255) Waste Valorization

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-228B

Michael T. Timko, Chair
Justinus Satrio, Co-Chair

Sponsored by: Forest and Plant Bioproducts Division

8:00 Paper 255a: Fabrication of Waste Biomass-Derived Aerogel Using Zinc Chloride Salt Hydrate — ***Mairui Zhang***, *Yang Liao, Daniel Fougnier, Ivan Gitsov, Gyu Leem, Xuejun Pan, Jeong Jae Wie, Chang Geun Yoo*

8:15 Paper 255b: Evaluation of Physical and Morphological Alteration of Seaweed Char with Varying Activation Parameters and Corresponding Fate on Cationic Dye Adsorption — ***Cadianne Chambers***, *Toufiq Reza*

8:30 Paper 255c: Uncovering the Effect of Mechanochemical Pretreatment on Biocrude Yields and Chemical Mechanism of Lignocellulosic HTL — ***Heather LeClerc***, *Alex Maag, Geoffrey Tompsett, Michael T. Timko, Andrew R Teixeira*

8:45 Paper 255d: Structure-Property Relationships of Lignin-Thermoplastic Polyurethane Composites — ***Seoku Lee***, *Heeeun Lee, Mandeep Poonia, Kijoon Yang, Kwangho Kim, Chang Geun Yoo, Jeong Jae Wie*

(256) Developments in Shale Gas and Natural Gas

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, W-103A

M R Riazi, Chair
Wade Vincent Wilding, Co-Chair
John McLennan, Co-Chair

Sponsored by: Fuels and Petrochemicals Division

8:00 Paper 256a: Reservoir Quality Indicators and Relative Thermal Maturity Classification Using Image-Based and Bulk Rock Characterization — ***Shannon Eichmann***, *David Jacobi, Poorna Srinivasan, Jennifer Rodriguez*

8:20 Paper 256b: Benefits of Removing Nitrogen before the Cold Section in Baseload LNG Plant — ***Ajinkya Pal***, *Iftekhar Karimi, Easa Al-Musleh*

8:40 Paper 256c: Modeling Uncertainty and Impact of Non-Darcy Flow Regimes on Unconventional Well Performance. — ***Harun Ates***, *Shannon Eichmann, Kanhaiyalal Patel, Ravi Vaidya, Rabah Mesdour*

9:00 Paper 256d: Elucidation of Non-Catalytic Ethylene Polymerization Reactions through Computational Study — ***Alexander Shaw***, *Grant Marsden, Linda Broadbelt*

9:20 Paper 256e: Functionalized Iron Oxide (Fe_3O_4) Nanoparticles As a New Type of Recyclable Hydrate Dispersant — ***Yuanxing Zhang***, *Ning Wu, Amadeu Sum*

9:40 Paper 256f: Techno-Economic Analysis of Natural Gas Transportation Technologies By Aspen Plus and Engineering Economic Modelling — ***Bhavikkumar Mahant***, *Omkar Singh Kushwaha, Rajnish Kumar*

(257) Topical Plenary: Frontiers in Green Process and Product Engineering (Invited Talks)

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-229AB

Wei Liu, Chair
Kevin Whitty, Co-Chair
Jian Liu, Co-Chair

Sponsored by: Green Process and Product Engineering

8:00 Paper 257a: *Low-Cost Waste Feedstock Conversion to Sustainable Aviation Fuel* — ***Karthikeyan Ramasamy***, *Michael R. Thorson*

8:35 Paper 257b: Process Systems Engineering Contributions to Flexible Carbon Capture — ***Michael Baldea***, *Joan Brennecke, Kyeongjun Seo, Mark Stadtherr*

9:10 Paper 257c: Process Engineering in Developing and Commercializing Breakthrough Technologies for Sustainability — ***Yizu Zhu***

(259) Advanced Manufacturing of Composites: 3D and 4D Composites

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-121A

Dong Lin, Chair
Kenan Song, Co-Chair
Yang Yang, Co-Chair

Sponsored by: Composites

8:00 Paper 259a: Nano Composite Material Based Gas Diffusion Layer for Proton Exchange Membrane Fuel Cell — *Arunachala Kannan,* ***Shuchi Sharma***

8:15 Paper 259b: Coupling Rheometry and Computed Tomography to Study the Evolution of Voids during the Consolidation of CF/Pekk Composites — *Raphaël Arquier, Ilias Iliopoulos, Gilles Régnier,* ***Guillaume Miquelard-Garnier***

8:35 Paper 259c: Postprint Microwaves Processing to Enhance Mechanical Performance of Carbon-PEEK Composites — *Jia-Ruey Ai,* ***Bryan Vogt***

8:55 Paper 259d: Synthesis of Ag-Fe/ZnO Composites By Sol Gel Method: Evaluation of Photocatalytic and Antibacterial Activities — ***Muneer Ba-Abbad***

9:15 Paper 259e: High-Precision Composite 3D Printing with High-Resolution Layer Control — ***Dharneedar Ravichandran,*** *Kenan Song*

9:30 Paper 259f: Electrochemical Synthesis of Bulk Copper-Carbon Nanotube Composites — ***Crystal Owens,*** *Gareth H. McKinley, A John Hart*

9:45 Paper 259g: Fabrication of a Novel Carbon/Carbon Composite with Micro-Channels for Concentrated Solar Power Gas Receivers — ***Jose Cordeiro Jr.,*** *Rachel Davis, Hema Ramsurn, Daniel W. Crunkleton, Todd Otanicar, Michael Keller*

10:00 Paper 259h: Next-Generation of Thermoplastic Nanocomposites Via Electromagnetic Processing — ***Byron Villacorta, Utsab Roy Ayan, Madara Karunarathna***

10:15 Paper 259i: *Detailed Characterization and Fabrication of 3D Printed Graphene/Polymer Structures for Heterojunction-Devices with MoS2 and Other 2D Nanomaterials* — ***Deisy Cristina Carvalho Fernandes***

(260) Area Plenary: Emerging Areas in Polymer Science and Engineering I (Invited Talks)

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-121B

Shudipto K. Dishari, Chair
Michelle Calabrese, Co-Chair
Siamak Nejati, Co-Chair

Sponsored by: Polymers

8:00 Paper 260a: Sequence Effects in Calcium-Responsive Biopolymers — *Marina P. Chang, Alana P. Gudinas, Winnie Huang,* ***Danielle Mai***

8:30 Paper 260b: Understanding the Role of Conjugated Polymer's Dynamics for Device Stability — ***Xiaodan Gu,*** *Luke Galuska*

9:00 Paper 260c: Radical-Mediated Ring Opening Photopolymerization for Semi-Crystalline Thermoplastic Additive Manufacturing — ***Timothy F. Scott,*** *Alex J. Commisso, Gopal R. Sama*

9:30 Paper 260d: *Design for Manufacturability: Linking Formulation to Processability in Electrospinning* — *Elena Ewaldz, Haley Carroll,* ***Blair Brettmann***

10:00 Paper 260e: Tackling the Plastics Waste Challenge Via an Interdisciplinary Framework: Catalytic Innovations, Material Complexity, and Sustainable Polymer Design — ***LaShanda Korley***

(261) Biomaterial Scaffolds for Tissue Engineering I

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-122B

Amol Janorkar, Chair
Mario Moisés Álvarez, Co-Chair
Metin Uz, Co-Chair
Gulden Camci-Unal, Co-Chair

Sponsored by: Biomaterials

8:00 Paper 261a: Biomaterials That Breathe for Regenerative Engineering — ***Gulden Camci-Unal***

8:18 Paper 261b: Protein-Loaded Self-Assembled Silk Fibroin Coatings for Sustained Drug Delivery from PLLA Electrospun Scaffold Surfaces — ***Tanner D. Fink,*** *Jessica L. Funnell, Ryan J. Gilbert, Runye Zha*

8:36 Paper 261c: High Throughput and Simple Fabrication of Compartmentalized Hydrogel Microbeads for Tissue Culture Applications — ***Carlos Fernando Ceballos-González,*** *Edna Johana Bolívar-Monsalve, Claudia Alarcón-López, María José Santoyo-de León, Grissel Trujillo-de Santiago, Mario Moisés Álvarez*

8:54 Paper 261d: Monocyte Recruitment for Vascular Tissue Regeneration — ***Bita Nasiri,*** *Tai Yi, Randall Smith Jr., Yulun Wu, Christopher Breuer, Stelios Andreadis*

9:12 Paper 261e: Biodegradable and Implantable Platform for Wireless Electrical Stimulation of Neural Stem Cells — ***Andrea Zuccaro,*** *Naomi Addai Asante, Metin Uz*

9:30 Paper 261f: 3D Printable Shape Memory Polymer Foams from Thiol-Ene and Thiol-Epoxy "Click" Reactions for Biomedical Tissue Scaffolding Implants — ***Andrew Weems***

9:48 Paper 261g: Polyurethane-Hydroxyapatite Scaffolds for Bone Regeneration — *Henos H. Tadesse,* ***Aaron S. Goldstein***

10:06 Paper 261h: Biodegradable Nanofiber Scaffold As Remotely Controlled and Self-Powered Electrical Stimulator for Enhanced Bone Regeneration — ***Ritopa Das,*** *Thanh Nguyen*

(262) Biomaterials: Graduate Student Award Session

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-121C

Kyle Lampe, Chair
Ramya Kumar, Co-Chair
Nisarg Shah, Co-Chair

Sponsored by: Biomaterials

8:00 Paper 262a: Graduate Student Award Session: Substrate Stiffness Regulates Microglial Phenotype and Function — ***Timothy Hackett,*** *Srivatsan Kidambi*

8:18 Paper 262b: Graduate Student Award Session: Kinetics and Thermodynamics of Peptide Binding and Peptide Release from Oxyntomodulin and Aib2-Oxyntomodulin Nano-Fibrils — ***Alireza Mohammad Karim,*** *Ana L. Gomes Dos Santos, Mark E. Welland*

8:36 Paper 262c: Graduate Student Award Session: Combining Tunable Biomaterials and Flow-Based Membrane Technologies for Improved Biomanufacturing of T Cell Therapies — ***Kartik Bomb,*** *Paige LeValley, Ian Woodward, Zaining Yun, Bryan P. Sutherland, Samantha Cassel, Emily Kurdzo, Jacob McCoskey, Kara Levine, Christina Carbrello, Abraham Lenhoff, Catherine Fromen, April Kloxin*

8:54 Paper 262d: Graduate Student Award Session: Glucose-Fueled Peptide Self-Assembly for Hypoglycemia Rescue — ***Sihan Yu,*** *Sijie Xian, Zhou Ye, Irawan Pramudya, Matthew Webber*

9:12 Paper 262e: Graduate Student Award Session: Supramolecular Reinforcement of Polymer–Nanoparticle Hydrogels for Modular Material Design — ***Giovanni Bovone,*** *Elia A. Guzzi, Stéphane Bernhard, Tim Weber, Dalia Dranseikiene, Mark Tibbitt*

9:30 Paper 262f: Graduate Student Award Session: A Biomimetic Hyaluronic Acid Hydrogel Models Mass Dormancy in Brain Metastatic Breast Cancer Spheroids — ***Raghu Vamsi Kondapaneni,*** *Lalita A. Shevde, Shreyas Rao*

9:48 Paper 262g: Graduate Student Award Session: Mimicking Biopolymer Structure in Synthetic Hydrogels for Model Extracellular Matrices — ***Logan D. Morton,*** *David A. Castilla-Casadiego, Ajay C. Palmer, Adrianne Rosales*

(263) Materials for Effective Energy Storage (Co-sponsored with Material Interfaces as Energy Solutions)

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-227A

Yuzhang Li, Chair
Matthew Panthani, Co-Chair
Andrej Lenert, Co-Chair
Carissa Eisler, Co-Chair

Sponsored by: Electronics and Photonics

8:00 Paper 263a: *High-Valent Redox Cathode Materials for Electrochemical Application* — ***Iwnetim Abate***

8:30 Paper 263i: Electrolyte Influence on Nonaqueous Electrochemical Conversion of Carbon Dioxide — ***Chibueze Amanchukwu***

9:00 Paper 263c: Galvanically Displaced Noble Metal Nanoparticles Onto Graphene-CNT Coated Ni-Foam Layered Double Hydroxide Composites for Energy and Storage Conversion Applications — ***Caspar Yi***, *Sean P. Rogers, Michael J. Williams, Nancy Astabie, Vesa Ibrahimi, Matthew Moellering, Tyler Komorowski, Alexander Liesen, Yash Joshi, Yong Joo, Deryn Chu, Preston Haney, Enoch Nagelli*

9:12 Paper 263d: Probing Solvation Thermodynamics of Lithium Battery Electrolytes Using Potentiometric Methods — ***Sang Cheol Kim***, *Yi Cui*

9:24 Paper 263e: Ionic Liquid Battery Electrolytes with Functional Organic Cations to Enhance Lithium Mobility — ***Bingchen Wang***, *Matthew Gebbie*

9:36 Paper 263f: The Connection between Slurry Rheology and Electrochemical Performance of Graphite Anodes in Lithium-Ion Batteries — ***Joseph Sullivan***, *Arijit Bose*

9:48 Paper 263g: Fabrication of ZSM-5 Zeolite Nanosheet Tiled Membranes on Macroporous Polymer Substrates As Ion Separators for Redox Flow Batteries — ***Landysh Iskhakova***, *Zishu Cao, Xinhui Sun, Junhang Dong*

10:00: Break

10:12 Paper 263b: Solvent-Based Synthesis and Integration of Engineered Nanomaterials in Energy Storage Devices — *Guesang K. Lee,* ***Vincent Holmberg***

(264) Synthesis and Application of Inorganic Materials I: Synthesis

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-122A

Wei Fan, Chair
Praveen K. Thallapally, Co-Chair

Sponsored by: Inorganic Materials

8:00 Paper 264a: Novel Three-Phase Zeolite Intergrowth (CHA/ERI/OFF) Control with a Single Organic Structure-Directing Agent (SDA) — ***Soonhyoung Kwon***, *Tom Willhammar, Daniel Schwalbe-Koda, Rafael Gomez-Bombarelli, Elsa Olivetti, Manuel Moliner, Yuriy Roman*

8:15 Paper 264b: Studying the Synthesis of Hierarchical Siliceous Zeolites By Post Synthetic Zeolite Surfactant-Templating — ***Kaivalya Gawande***, *Wei Fan*

8:30 Paper 264c: Insights into Faujasite Crystallization through in Situ Imaging — ***Zhiyin Niu***, *Rishabh Jain, Madhuresh Choudhary, Jeffrey Rimer*

8:45 Paper 264d: Roles of Metal Cations in Static and Continuous Synthesis of Phillipsite and Tobermorite — ***Juan Carlos Vega-Vila***, *Advait Holkar, Ross A. Arnold, Samanvaya Srivastava, Gaurav Sant, Dante Simonetti*

9:00 Paper 264e: Template-Free Preparation of EMT Zeolite and Its Coatings — *Zulfiye Dagli,* ***Cigdem Atalay-Oral***, *Melkon Tatlier*

9:15 Paper 264f: Understanding the Formation Mechanism of Hierarchically Porous Petrified Hollow Fiber Membranes — ***Ching-En Ku***, *Chen Zhang*

9:30 Paper 264g: Fabrication & Modeling of Percolation Aided Continuous Coating of Metal Organic Frameworks on Porous Substrates — ***Rajan Bhawnani***, *Rohan Sartape, Aditya Prajapati, Prem Podupu, Paria Coliaie, Meenesh Singh*

9:45 Paper 264h: Improving Low-Temperature CH_4 Oxidation Performance with High-Silica Pd/CHA Zeolite Catalysts — ***Jingzhi Liu***, *Tala Mon, Eleni Kyriakidou, Viktor Cybulskis*

10:00 Paper 264i: Design and Synthesis of Zeolite Catalyst for Production of Hydrocarbons from Methane Via Methanol — *Kengo Nakamura, Shuhei Yasuda, Peipei Xiao, Yong Wang, Ryota Osuga, Atsushi Muramatsu,* ***Toshiyuki Yokoi***

(265) Area Plenary: Carbon Nanomaterials (Invited Talks)

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, W-104B

Anju Gupta, Chair

Sponsored by: Carbon Nanomaterials

8:00 Paper 265a: We Can Use Carbon to Decarbonize—and Get Hydrogen for Free — ***Matteo Pasquali***

8:25 Paper 265b: Deconstructing Proton Transport through Atomically Thin Monolayer CVD Graphene Membranes — ***Piran Kidambi***

8:50 Paper 265c: Developing Carbon Nanomaterials Electrocatalysts for Active and Selective Carbon Dioxide to Target Products Conversion — ***Jingjie Wu***

(266) Plenary Session for Nanomaterials for Energy Applications (Invited Talks)

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, W-104A

Yong L. Joo, Chair
Seung Soon Jang, Co-Chair

Sponsored by: Nanomaterials for Energy Applications

8:00 Paper 266a: Combining Quantum Chemistry with Multiscale Atomistic Reactive Simulations to Develop New Nanomaterials for Energy Applications — ***William Goddard III***

8:50 Paper 266b: Tailoring Processes and Assembly of Polymer, Ceramic and Graphenic Materials for Electrochemical Energy Storage Applications — ***Yong Joo***

9:40 Paper 266c: Channel Engineering in Solid Polymer Electrolytes for Electrochemical Energy Storage and Conversion Devices — ***Paul Kohl***

(267) Mixing in Multiphase Systems

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-227C

Ravindra Aglave, Chair
Clara Gomez, Co-Chair

Sponsored by: North American Mixing Forum

8:00 Paper 267a: On the Dispersion Dynamics of Liquid-Liquid Surfactant-Laden Flows in Static Mixers — ***Juan Valdes***, *Fuyue Liang, Lyes Kahouadji, Seungwon Shin, Jalel Chergui, Damir Juric, Omar K. Matar*

8:30 Paper 267b: Numerical Simulation of Surfactant-Laden Emulsion Formation in a Stirred Vessel — ***Fuyue Liang***, *Juan Valdes, Lyes Kahouadji, Seungwon Shin, Jalel Chergui, Damir Juric, Omar K. Matar*

9:00 Paper 267c: The Transition to Aeration in Turbulent Two-Phase Mixing in Stirred Vessels — ***Lyes Kahouadji***, *Fuyue Liang, Juan Valdes, Seungwon Shin, Jalel Chergui, Damir Juric, Omar K. Matar*

9:30 Paper 267d: Multiscale Modelling of Food Emulsions: From Molecules to Mixing Equipment — ***Marco Ferrari***, *Alessio Lombardo Pontillo, Antonio Buffo, Gianluca Boccardo, Marco Vanni, Daniele Marchisio*

10:00 Paper 267e: Rapid Mixing in Microfluidic Devices with Induced-Charge Electro-Osmosis for Improved Control over Precipitation Reactions — ***Dishika Gupta**, Baggie W. Nyande, Kiran Mathew Thomas, Fei Li, Andrew T.C. Mak, Richard Lakerveld*

(268) Theory, Modeling and Simulation of Nuclear Chemical Processes I

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, W-102C

Valmor de Almeida, Chair
Maximilian Gorensek, Co-Chair

Sponsored by: Nuclear Engineering Division

8:00 Paper 268a: Development of Extraction Process Flowsheets for Recovery of Uranium from Used Nuclear Fuel — ***Candido Pereira**, Laura Maggos, Jackie Copple*

8:21 Paper 268b: Nuclear Nonproliferation Stewardship Program - Uranium S&T Center — ***Jared Johnson***

8:42 Paper 268c: Modeling and Simulation for Safeguards at Nuclear Waste Reprocessing Facilities — ***Anna Taconi**, Benjamin Cipiti, Nathan Shoman*

9:03 Paper 268d: Digital Network Twin of the UMass Lowell Research Reactor Facility — ***Valmor de Almeida**, Sukesh K. Aghara, Joseph Boffie*

9:24 Paper 268e: The Atkau Nuclear Power Plant and Its Relevance to Models of Nuclear Hydrogen — ***CT Callaway**, Nicholas Brown*

9:45 Paper 268f: Properties of Tri-Butyl-Phosphate from Polarizable Force Field MD Simulations — ***Faranak Hatami**, Valmor de Almeida*

10:06 Paper 268g: Radioisotope Target Dissolution Modeling and Simulation — ***Michael Dion**, Valmor de Almeida, David Abrecht, Andrew Conant, Ken Dayman, Riley Hunley, Richard Reed, Charles Weber*

(269) Novel Nanoparticles and Nanostructured Materials for Pharmaceuticals and Medical Applications

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, W-106A

Abhinav Sannidhi, Chair

Sponsored by: Nanoparticles

8:00 Paper 269b: "Ringing" Breast Tumors with Ligand-Specific X-Ray Contrast Agents and Spectral CT — *Kalyan Ramesh, Alice Truong, Mary Ruskowski, **Manos Gkikas***

8:21 Paper 269c: Platinum Nanoparticles Encapsulated within PLGA, Treatment for TNBC, an *in Vitro* and *In Vivo* study — ***Aida López Ruiz**, Kathleen McEnnis*

8:42 Paper 269d: A Personalized Approach Towards the Delivery of Itraconazole Nanocrystals Onto Contact Lenses Using Inkjet Printing — ***Carolin Tetyczka**, Kira Brisberger, Martin Reiser, Manuel Zettl, Ramona Jeitler, Christina Winter, Dagmar Kolb, Gerd Leitinger, Martin Spörk, Eva Roblegg*

9:03 Paper 269e: Indocyanine Green J-Aggregate and Anticancer Drug Loaded Polymersomes for Photoacoustic Image-Guided Drug Delivery — ***Ceren Atila Dincer**, Mohammed Kawelah, Sangheon Han, Thomas Truskett, Konstantin V. Sokolov, Keith P. Johnston*

9:24 Paper 269f: Eradication of Antibiotic-Resistant Biofilms By Hyperthermia Using Superparamagnetic Iron Oxide Nanoparticle Films — ***Shaquib Rahman Ansari**, Georgios Sotiriou, Alexandra Teleki*

9:45 Paper 269g: Thermal Decomposition Synthesis of Iron Oxide Nanoparticles in a Precision Machined Reactor with Enhanced Gas-Liquid Mass Transfer for Magnetic Particle Imaging (MPI) — ***Ambar C. Velazquez-Albino**, Kaitlyn King, Grace Li, Carlos Rinaldi-Ramos*

10:06 Paper 269h: A Simulation-Based Thermodynamic Model to Pre-Screen Peptide Amphiphile Micelle Vaccines — ***Luke Kruse**, Bret Ulery, Karl Hammond*

(270) Particulate Mixing and Segregation

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, W-106B

Yu Liu, Chair
Deeksha Jain, Co-Chair

Sponsored by: Solids Flow, Handling and Processing

8:00 Paper 270a: Scaling up Segregation Learnings in Industrial Bin Flow — ***Alexander M. Fry**, Jason A. Stamper, Christopher G. Stoltz, John P. Hecht*

8:18 Paper 270b: Drag on a Sphere in Granular Shear Flows — *Lu Jing, Julio M. Ottino, Paul B. Umbanhowar, **Richard Lueptow***

8:36 Paper 270c: Flow and Segregation of a Mixture of Passive and Responsive, Magnetically-Driven Rotating Particles — *Samuel Wilson-Whitford, Jinghui Gao, William Buckley, David Kramer, **James Gilchrist***

8:54 Paper 270d: Experimental Investigation of Segregation in a Rotating Cylinder with Non-Spherical Particles — ***Sunil Kumar**, Anshu Anand*

9:12 Paper 270e: DEM Study of Non-Spherical Ellipsoidal Particles in a Vertically Vibrated Packed Bed System — ***Salma Khatoon**, **Anshu Anand***

9:30 Paper 270f: A Particle-Force Based Theory for Size Segregation of Binary Granular Mixtures — ***Anurag Tripathi**, Alok Kumar, Mohit Nema, Devang Khakhar*

9:48 Paper 270g: Time Dependent Size Segregation of Binary Granular Mixtures Flowing over a Chute — ***Soniya Kumawat**, Vishnu Kumar Sahu, Satyabrata Patro, Anubhav Majumdar, Anurag Tripathi*

10:06 Paper 270h: Investigation of Segregation Effect on the Packing Fraction for Density Estimation — ***Salvatore Pillitteri**, **Filip Francqui**, **Aurelien Neveu**, **Geoffroy Lumay***

(271) Session honoring lifetime achievement of Madhava Syamlal

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, W-106C

Sreekanth Pannala, Chair
Sankaran Sundaresan, Co-Chair
Charles E. A. Finney, Co-Chair

Sponsored by: Fluidization and Fluid-Particle Systems

8:00 Paper 271a: From Mfix to Ccsi to Exa: A Retrospective on the Career of Madhava Syamlal — ***David Miller***

8:18 Paper 271b: Don't get stuck: A DEM model for particle-particle cohesion using simple bulk experiments — ***Christine Hrenya***

8:36 Paper 271c: Modeling and Numerical Simulation of Concentrated Solar EnergyStorage and utilization using Packed and Fluidized bed Systems — ***Zeyuan Gao**, Javad Abbasian, Hamid Arastoopour*

8:54 Paper 271d: Some insights from validation studies of CFD-DEM modeling for gas-solids flows from lab to commercial scale — ***Tingwen Li***

9:12 Paper 271e: An assessment of drag models for predicting fluidized beds with two-fluid and multiphase particle-in-cell frameworks — ***Casey LaMarche**, Jia Wei Chew, Raymond Cocco*

9:30 Paper 271f: Gas-Solid Flow Models Based on the Kinetic Theory of Granular Flows: What Have We Learned Since MFIX Version 1? — ***Rodney Fox***

9:48 Paper 271g: Modeling Multiphase Flow Reactor Systems with Gas–Particle Reactions — ***Charles E. A. Finney***

10:06 Paper 271h: Particle transport during dry powder inhalation — *Mostafa Sulaiman, Xiaoyu Liu, **Sankaran Sundaresan***

(272) Continuous Processing in Drug Substance: Modelling & Simulation

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-123

Luke Rogers, Chair
Jasmine Rowe, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

8:00 Paper 272b: Digital Twin Development for Continuous Drug Manufacturing — ***Busuyi Adebayo**, Syed Ahmed, Rob Guenard*

8:21 Paper 272c: A Modeling Based Comparison for Two Continuous Synthesis Routes of Carbamazepine — ***Matthew Glace**, Wei Wu, Thomas Roper, Adil Mohammad*

8:42 Paper 272d: Integrated Flowsheet Model of Continuous API Manufacturing Process and Its Applications for Dynamic Optimization and Control — ***Ravendra Singh**, Fernando Muzzio*

9:03 Paper 272e: Process Development and Scale-up of Continuous Hydrogenation from Lab Scale to Pilot Plant in a Trickle Bed Reactor — ***Onkar Manjrekar**, Christopher Vitale, Greg Storer, Brian Kotecki, Narendrabh Patel, Duygu Gerceker, Jie Chen, Moiz Diwan*

9:24 Paper 272f: Tracking Lot Genealogy in Continuous Drug Substance Manufacturing Processes through Mechanistic Modeling — ***Meera Mahadevan***

9:45 Paper 272g: A Step-By-Step Strategy for Modeling, Scaling-up, and Control of Aspirin Production in a Continuous Tubular Antisolvent Crystallizer Under Ultrasound — ***Symeon Savvopoulos**, Mohammed N. Hussain, Spyridon Voutetakis, Tom Van Gerven, Dimitris Ipsakis, Simon Kuhn*

(273) Facilities of the Future (Invited Talks)

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-122C

Moiz Diwan, Chair
Jasmine Rowe, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

8:00 Paper 273b: Pharmacy on Demand: A Case of Arrested Development or Flourishing Adolescence — ***Luke Rogers***

8:25 Paper 272a: Facility Design for Continuous Clinical Supply Facilities and Laboratories — ***Christopher Vitale**, Jie Chen, Moiz Diwan, James Ratway*

8:50 Paper 273c: A Hybrid Liquid Phase Peptide Synthesis (LPPS) Facility — ***Darragh McDonagh***

9:15 Paper 273d: Digitalization in Pharmaceutical Development — ***Jaquan Levons***

9:40 Paper 273a: Modular Flexible Manufacturing - Enabling and Accelerating Specialty Product Development and Commercialization — ***Athanas Koynov**, Celeste Frankenfeld*

10:05 Paper : A Digital Paradigm for mRNA Vaccine Development — ***Aparajita Dasgupta***

(274) Challenges and Best Practices in Technology Commercialization

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-221C

John Peragine, Chair
Ha Dinh, Co-Chair

Sponsored by: Technology Transfer and Manufacturing

8:00 Paper 274a: Challenges of Minor Impurities in Process Development — ***Glenn Graham**, **Raymond Rooks***

8:25: Break

8:50 Paper 274c: Successful Commercialization Involves More Than a Great Idea — ***John Gohndrone***

9:15 Paper 274d: Successful Process Technology Development Strategies for Commercial Success — ***Michael Telgenhoff***

9:40 Paper 274e: Never Let a Good Crisis Go to Waste: RAPID RACER AMPD and the Opportunity to Accelerate Modular Process Development — ***Cheryl Teich**, John Dever, Mike Burgess, Robert Nunley, Ignasi Palou Rivera, Nima Yazdanpanah*

(275) Process Intensification - Novel Reactors

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-222A

Robert Broekhuis, Chair
Kishori Deshpande, Co-Chair

Sponsored by: Process Intensification & Microprocess Engineering

8:00 Paper 275a: Aiding Catalysis with Membrane Reactor Design: Optimization of Hierarchical Membrane/Catalyst Systems for the Oxidative Coupling of Methane — ***James Wortman***

8:25 Paper 275b: Large Eddy Simulation of a Rotor Stator Spinning Disk Reactor — ***Christianus Hop**, Rick Jansen, Matthijs Besten, Arnab Chaudhuri, John van der Schaaf*

8:50 Paper 275c: Intensifying the Recovery of Carboxylic Acids from Fermentation Broths Via Reactive Extraction inside the Membrane-Assisted Spinning Disc Reactor — ***Brandon Leal Perez**, Fausto Gallucci, John van der Schaaf*

9:15 Paper 275d: Scalable on-Demand Production of Purified Diazomethane Suitable for Sensitive Catalytic Reactions — ***Jillian Sheeran**, M. Grace Russell, Kiersten Campbell, David D. Ford, Yuan-Qing Fang, Matthew Bio, Christopher P. Breen, Anamika Datta, Scott J. Hecker, Serge Boyer*

9:40 Paper 275e: Reactive CFD-DEM Simulations of Oxidative Coupling of Methane in a Gas-Solid Vortex Reactor — ***Florian Wéry**, Laurien A. Vandewalle, Geraldine J. Heynderickx, Kevin Van Geem*

10:05 Paper 275f: Novel & Optimized Front Photocatalytic Reactor for Toxic Gas Removal: Compactness, Intensification, Efficiency — ***Youcef Serhane**, Abdelkrim Bouzaza, Dominique Wolbert, Aymen Amin Assadi*

(276) Area Plenary: Fundamentals and Applications of Adsorption and Ion Exchange

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-131C

Daniel Siderius, Chair
F Handan Tezel, Co-Chair

Sponsored by: Adsorption and Ion Exchange

8:00 Paper 276a: On the Use of the Dual Process Langmuir Model for Predicting Mixed Gas Isotherms of Methane, Ethane and Ethylene Binary and Ternary Mixtures on Activated Carbon — ***Armin Ebner**, Jaclyn Couch, James A. Ritter*

8:18 Paper 276b: Comparison of Heterogeneous Langmuirian Models for Representation of Unary, Binary, and Ternary Adsorbate Systems at Adsorption Equilibria — *Michael D. Sees, Yinka Otulana, **Usman Hamid**, Chau-Chyun Chen*

8:36 Paper 276c: On the Use of a New Kinetic Model in a Cyclic Adsorption Process Simulator for Kinetically Limited Gas Separations — ***Sulaimon Adegunju**, Pravin B. C. A. Amalraj, Armin Ebner, James A. Ritter*

8:54 Paper 276d: Understanding the Break-through Curve Measurement When Adsorption Is Fast — ***Robert DeJaco**, Paul N. Patrone, Anthony J. Kearsley*

9:12 Paper 276e: Aspects of Gas Storage: Effect of Confinement on Supercritical Adsorption Behaviour — *Simon Eder, **Matthias Thommes***

9:30: Intermission

9:48: Break

10:06 Paper 371q: Degradation of Reactive Black 5 Dye Using Nanostructured Carbon Adsorbents — *Robert Haxhari, Kevin Zheng, Tyler Zmarzlak, Aldo Bushati, Taejin Kim, Yizhi Meng,* ***Steve Nitodas***

(277) Honorary Session for Prof. Suzana Nunes II

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-131B

Dibakar Bhattacharyya, Chair
Isabel Escobar, Co-Chair
Lakshmeesha Upadhyaya, Co-Chair
Cristiana Boi, Co-Chair

Sponsored by: Membrane-Based Separations

8:00 Paper 277a: Bridging the Interfacial Gap in Mixed-Matrix Membranes for Precise Molecular Sieving in Organic Solvents — ***Gyorgy Szekely***

8:20 Paper 277b: Membrane-Based Fractionation of Complex Mixtures — ***Ryan P. Lively***

8:40 Paper 277c: Development of High-Performance Polymeric Membrane for Natural Gas Dehydration — ***Eyad Qasem****, Suzana Nunes*

9:00 Paper 277d: Cross-Linked Block Copolymer Membranes — ***Radoslaw Gorecki****, Sandra Aristizabal Guerrero, Saibal Bhaumik, Konstantinos Ntetsikas, Nikos Hadjichristidis, Suzana Nunes*

9:20 Paper 277e: Polymeric Membranes for H_2 Separation — ***Tai-Shung Chung***

9:40 Paper 277g: Realisation of the Potential of Practical Graphene Oxide Membranes for Molecular Separations — ***Mainak Majumder***

10:00 Paper 277f: Effect of Packing Nonuniformity on the Performance of Hollow Fiber Membrane Gas Separation Modules Fabricated from Fiber Tows — *Lili Sun, Grigorios Panagakos,* ***Glenn Lipscomb***

(278) Membranes for CO_2 Capture I

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-132A

Nitesh Bhuwania, Chair
Winston Ho, Co-Chair
Junyi Liu, Co-Chair

Sponsored by: Membrane-Based Separations

8:00 Paper 278a: Integrated Facilitated Transport Membrane Modules for Highly Selective Syngas Purification and Carbon Capture — ***Yang Han****, Yutong Yang, Ruizhi Pang, W.S. Winston Ho*

8:21 Paper 278b: Hydrogen-Sieving Zeolitic Films By Filter Deposition on Porous Polymeric Support — ***Kumar Varoon Agrawal****, Xuekui Duan*

8:42 Paper 278c: Supramolecular Polymer Networks of Ion-Coordinated Polybenzimidazole for High-Temperature H_2/CO_2 Separation — ***Leiqing Hu****, Shouhong Fan, Liang Huang, Vinh Bui, Thien Tran, Sankhajit Pal, Yifu Ding, Mark Swihart, Haiqing Lin*

9:03 Paper 278d: Poly(4-vinylpyridine)-Based Catalytic Membranes for Integrated CO_2 Capture and Conversion — ***Casey O'Brien****, Renxi Jin, Hui Xu, Justin Easa, Sarah Pate*

9:24 Paper 278e: Molecularly Mixed Nanocomposite Membranes Based on High-Performance Commercial Polymer Blends for Efficientpre-Combustion CO_2 Capture — ***Fan Feng****, Ji Wu, Can-Zeng Liang, Martin Weber, Sui Zhang, Tai-Shung Chung*

9:45 Paper 278f: A Facilitated Transport Membrane Composed of Restricted Ionic Liquid in Graphene Oxide/Single Walled Carbon Nanotube Framework for Efficient Carbon Capture — ***Dinesh Behera****, Bratin Sengupta, Huazheng Li, Shiguang Li, Miao Yu*

10:06 Paper 278g: Water-Gas Shift Reaction with CO2 Capture in Ceramic-Carbonate Dual-Phase Membrane Reactor at High Temperatures and Pressures — ***Oscar Ovalle Encinia****, Jerry Lin*

(279) Nucleation and Growth I

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-131A

Meenesh Singh, Chair
Venkateswarlu Bhamidi, Co-Chair
Baron Peters, Co-Chair

Sponsored by: Crystallization and Evaporation

8:00: Introductory Remarks

8:03 Paper 279a: Non-Equilibrium Kink Density Model for Organic Molecular Crystals Containing Two Growth Units — ***Neha Padwal****, Michael F. Doherty*

8:32 Paper 279b: Growth Mechanism of Penta-Twinned Ag/Cu Nanowires: Multiscale Theory — ***Jianming Cui****, Junseok Kim, Kristen Fichthorn*

9:01: Break

9:30 Paper 279d: A Mathematical Model to Describe the Oriented Attachment of Molecules in Crystal Growth. — ***Ravi Kumar Reddy Addula****, Baron Peters*

9:59 Paper 279e: Influence of Transient Nucleation Phenomena on Induction Time at Low Supersaturation — ***Venkateswarlu Bhamidi****, Brendan P. Abolins*

10:28: Concluding Remarks

(280) Water Treatment, Desalination, and Reuse I

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-130

Isabel Escobar, Chair
Milad Esfahani, Co-Chair
William Phillip, Co-Chair

Sponsored by: Membrane-Based Separations

8:00 Paper 280a: Rapidly Ordered Block Copolymer Membranes with Tunable Pore Sizes for Wastewater Treatment — ***Kshitij Sharma****, Khadar Basha Shaik, Maninderjeet Singh, Chenhui Zhu, Mohammad Hassan, Alamgir Karim*

8:21 Paper 280b: Effect of Dehydration on RO Performance and Antifouling in Fully Aromatic Polyamide Membranes Containing Functionalized Cellulose Nanocrystals (CNCs) — ***Connor Farrell****, Ethan D. Smith, Keith Hendren, Earl J. Foster, Stephen Martin*

8:42 Paper 280c: Engineering Reduced Graphene Oxide Membrane Via in-Situ Peracetic Acid Etching to Achieve Excellent Water Permeance for Highly Efficient Dye Recovery — ***Erda Deng****, Kai Chen, Haiqing Lin*

9:03 Paper 280d: MIL-100 (Fe) Functionalized Thin-Film Nanocomposite Membranes for Enhanced Removal of Uncharged Urea from Water — ***Tin Le****, Milad Esfahani*

9:24 Paper 280e: Self-Regulating Behavior of a Pilot Scale Forward Osmosis-Reverse Osmosis Hybrid System — ***Jeffrey McCutcheon****, Noah Ferguson, Colin Fitzsimonds, Nicole Beauregard, Maqsud R. Chowdhury, Mayur Ostwal, Ranjan Srivastava*

9:45 Paper 280f: Multilayered Covalent Organic Framework Membranes Made By Sequential Interfacial Polymerization for Desalination — ***Xiaoli Ma****, Miguel Angel Jaimes, Ho Kuan Yu, Zhiqin Qiang, Weiling Xia, Rachel Clark*

10:06 Paper 280g: Post-Synthesis Modification of Polyamide Reverse Osmosis Membranes Via Diamines for Enhanced Urea Rejection — ***Shahriar Habib****, Madison Wilkins, Steven Weinman*

(281) Concentrated Solar Power Generation and Chemical Processing I

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-226C

Christopher Muhich, Chair
Alexandre Yokochi, Co-Chair
Wojciech Lipinski, Co-Chair
Nick AuYeung, Co-Chair
Ashley Pennington, Co-Chair

Sponsored by: Sustainable Energy

8:00 Paper 281a: Development and Testing of a High-Temperature Heat Recovery System for a Solar Redox Reactor — ***Alon Lidor***, *Leo Zimmermann, Pit Reckinger, Philipp Haueter, Aldo Steinfeld*

8:18 Paper 281b: Pressure Swing Redox Processing to Split Water and/or Carbon Dioxide — ***Justin Tran***, *Kent J. Warren, Alan Weimer*

8:36 Paper 281c: Automation and Parametric Study of a Solar Fuel System for the Thermochemical Production of Syngas from H_2o and CO_2 — ***Remo Schäppi***, *Vivien Hüsler, Aldo Steinfeld*

8:54 Paper 281d: Experimental Performance of Water-Splitting Photo-Electrodes Under High Solar Concentration — ***Isaac Holmes-Gentle***, *Franky Bedoya-Lora, Sophia Haussener*

9:12 Paper 281e: Metal Ferrite and Ceria Composites for Solar Thermochemical Fuel Production — ***Aniket Patankar***, *XiaoYu Wu, Wonjae Choi, Harry Tuller, Ahmed F. Ghoniem*

9:30 Paper 281f: La and Yb Incorporated Zr-Doped Ceria for Solar Thermochemical CO_2 Splitting: Thermodynamics and Oxidation Kinetics Study — ***Kangjae Lee***, *Nicole Knoblauch, Christos Agrafiotis, Mathias Pein, Martin Roeb, Christian Sattler*

9:48 Paper 281g: Experimental Evaluation of Thermal Energy Storage Using the Sorption-Assisted Boudouard Process — ***Alexandre Yokochi***, *Riley Choquette, Benjamin Phillips, Annette von Jouanne*

10:06 Paper 281h: Demonstration of Sustainable Air Separation Via a Coupled PSA-Thermochemical System — *Dorottya Kriechbaumer,* ***Lena Klaas***, *Nicole Neumann, Martin Roeb, Christian Sattler*

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(282) Value-Added Biorefinery Co-Products

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-226B

Mark Mba Wright, Chair
Ana I. Torres, Co-Chair

Sponsored by: Sustainable Biorefineries

8:00 Paper 282a: Optimal Integrated Plant for Biodegradable Polymers Production — *Jose Enrique Roldán-San Antonio,* ***Mariano Martin***

8:15 Paper 282b: Combining Hydrogenolysis and Microbial Funneling to Produce 2-Pyrone-4,6-Dicarboxylic Acid from Lignocellulosic Biomass — ***Canan Sener***, *Miguel Perez, German Umana, Shamik Misra, Yaoping Zhang, Christos Maravelias, Steven Karlen, John Ralph, Timothy J. Donohue, Daniel R. Noguera*

8:30 Paper 282c: Catalytic Hydrothermal Liquefaction of Lignocellulosic Biomass for Fuels and Value-Added Products — ***Bharathkiran Maddipudi***, *Khang Huynh, Vinod Amar, Anuradha Shende, Rajesh Shende*

8:45 Paper 282d: Fractionation, Characterization and Value-Addition of Endocarp Lignin — *Makua Vin-Nnajiofor, Wenqi Li, Seth Debolt, Yang-Tse Cheng,* ***Jian Shi***

9:00 Paper 282e: Crustacean Shells Waste Valorization - a Tale of Two Processes — ***Filipa A. Vicente***, *Sónia P. M. Ventura, Bárbara M.C. Vaz, Inês L. D. Rocha, Ana C. R. V. Dias, Mario A. Torres Acosta, Uroš Novak, Blaž Likozar*

9:15 Paper 282f: Towards the Upscale Production of Diformylxylose As a Solvent and a Platform Chemical — ***Zezhong Li***, *Anastasia Komarova, Jeremy Luterbacher*

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(283) Applications of Data Science in Catalysis and Reaction Engineering

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-230

Bryan Goldsmith, Chair
Zachary Ulissi, Co-Chair
Hongliang Xin, Co-Chair

Sponsored by: Applications of Data Science to Molecules and Materials

8:00 Paper 283a: Predicting the Performance of Mesophase Formation and Properties of Mesophase Pitch Based on Experimental Investigation and Machine Learning — ***Wenjia Wang***, *Madison Cooley, Karissa Jolley, Robert M. Kirby, Eric Eddings*

8:20 Paper 283b: Deep Active Learning Enabled High-Throughput Catalyst Design for CO2 Electroreduction — ***Chen Honghao***, *Jiali Li, Xiaonan Wang*

8:40 Paper 283c: Bayesian Reaction Optimization of *Rac*-Lactide Polymerization Catalyzed By Aluminum Complexes — ***Yang Huang***, *Maverick Lin, Rong Tong, Hongliang Xin*

9:00 Paper 283d: Inferring Structure-Entropy Correlations of Zeolite-Adsorbate Interactions Using Monte-Carlo Simulations & Machine Learning — ***Christopher Rzepa***, *Srinivas Rangarajan*

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(284) Big Data and Machine Learning to Advance Medicine

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-126C

Karthik Shekhar, Chair
Varghese Kurian, Co-Chair

Sponsored by: Chemical Engineers in Medicine

8:00 Paper 284a: Data-Driven QSAR Modeling for the Iterative Identification of Chemical Motifs from Limited Data — ***Hyun-Seob Song***, *Chul Min Park, Soojin Jang, Jae Sun Kim, Hyung Chul Ryu, Hasoo Seong*

8:19 Paper 284b: Single Sequence Prediction of Protein Structure and Impacts on Computational Protein Design — ***Ratul Chowdhury***

8:38 Paper 284c: Hierarchical Graph-Based Representation Drives Prediction of Stapled Peptide Drug-like Properties — ***Marshall Case***, *Camille Bilodeau, Greg Thurber*

8:57 Paper 284d: Data-Driven Approach for the Prediction of MHC Class II Epitopes Using Oscillations of Physicochemical Properties — ***Hyeju Song***, *Christopher Kieslich*

9:16 Paper 284e: Automated Detection of Apoptotic Bodies in Label-Free Time-Lapse High-Throughput Microscopy Using Deep Convolutional Neural Networks — ***Kwan-Ling Wu***, *Melisa Martinez-Paniagua, Kate Reichel, Prashant Menon, Shravani Deo, Badrinath Roysam, Navin Varadarajan*

9:35 Paper 284f: Single-Cell Transcriptomic Analysis of Neural Development — ***Karthik Shekhar***

9:54 Paper 284g: Structure-Guided Functional Phylogenetic Trees of Human Channel Proteins and Kinases for Drug Discovery — ***Ratul Chowdhury***

10:13 Paper 284h: Machine Learning Enabled Cancer and Immune Cells Segmentation on Clinical Images — *Vidit Shah, Felicia Poynter,* ***Shachi Mittal***

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(285) 3D Printing of Functional Materials

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-221B

Monirosadat Sadati, Chair
Satish Nune, Co-Chair
Kuochen Tsai, Co-Chair

Sponsored by: 3D Printing

8:00 Paper 285a: Using Additive Manufacturing to Advance the Design of Water Treatment Devices — ***William Phillip***

8:30 Paper 285b: 4D Printing of Hydrogels Displaying Swelling-Induced Surface Wrinkling Patterns — ***Murat Guvendiren***

9:00 Paper 285c: Multiphoton Lithography of Organic Semiconductor Devices for 3D Printing of Flexible Electronic Circuits, Biosensors, and Bioelectronics — ***Mohammad Reza Abidian***

9:30 Paper 285d: 3D Synthetic Brain: Manufacturing, Challenges, and Fundamental Studies — *Lawrence Ray, Caleb Shaw, Terence C. Burns,* ***Dr. M. Rashed Khan***

9:45 Paper 285e: Additive Manufacturing of MOF Contactors for CO_2 Capture — ***Hannah Holmes***, *Wenying Quan, Simon C. Weston, Carter W. Abney, William J. Koros, Matthew Realff, Ryan P. Lively*

10:00 Paper 285f: Modeling of Sagging for 3D Printed Layers during the Curing Process — ***Andrey Filippov***, *Jeremy M. Lenhardt, Todd H. Weisgraber, Thomas S. Wilson, Fangyou Xie, Lemuel X. Perez Perez, Andrew L. Nguyen, Steven J. Guzorek, Hamed Z. Ammar*

(286) Future of Manufacturing and Emerging Technologies

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-221A

Qi Zhang, Chair
Yuncheng Du, Co-Chair

Sponsored by: Next-Gen Manufacturing

8:00 Paper 286a: Fusion of EEG and Eye-Tracking Based Metrics for Characterizing the Cognitive State of Control Room Operators — ***Mohd Umair Iqbal***, ***Babji Srinivasan***, ***Rajagopalan Srinivasan***

8:25 Paper 286b: Development and Application of Customized Symbols in PI Vision for KPI Monitoring Based on the Greenscope Methodology — ***Esmael Gadelha***, *Igor Guerra, Natalya A. B. Almeida, Beatriz Dantas, Fernando V. Lima,* ***Heleno Bispo***

8:50 Paper 286c: Design Space Exploration and Optimization for Additive Manufacturing through Rational Feature Engineering and Machine Learning — ***Alexander Summers***, *Q. Peter He*

9:15 Paper 286d: Images, Motion Capture, Three-Dimensional Modeling, and Haptics for Future Manufacturing — *Govanni Gjonaj, Renee O'Neill, Minhazur Rahman, Jacob Headley, Paloma Beacham, Samantha Cherney, Michael Williamson, Keshav Kasturi Rangan,* ***Helen Durand***

9:40 Paper 286e: Image Prediction for Model Predictive Control — ***Dominic Messina***, *Helen Durand*

10:05 Paper 286f: Real-Time Coordinating of Multiple Conveyor-Belt Tripper Car Positioning for Multi-Quality Stockpiles Towards the Mines of the Future — *Mohammed Yaqot,* ***Brenno Menezes***, *Robert Franzoi, Jeffrey D. Kelly*

(287) Field-Deployable Sensors

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-231A

Kevin Cash, Chair
Yixin Liu, Co-Chair

Sponsored by: Sensors for Sustainability

8:00 Paper 287a: Invited Talk: Field Deployable Sensor Arrays with Molecular Selectivity — ***Thomas Thundat***

8:40: Break

8:55 Paper 287c: Novel Field Deployable Sensors to Monitor How Dynamic Hydrology Shapes Nutrient and Element Transformations in a Great Lakes Coastal Estuary — ***Chelsea Monty-Bromer***, *Sai Prasanna Chinthala, Bukola Adesanmi, Zachary Cheney, Lauren Kinsman-Costello, John Senko, Joshua Davis*

9:10 Paper 287d: A Silica Nanofiber-Based Colorimetric Sensor for the Point-of-Use Detection of Polycyclic Aromatic Hydrocarbons in Water — ***Colton Duprey***, *Hadi Rouhi, Hannah Stumpft, Emily Linn, Sarah Veres, George Chen, Mark Elliott, Evan Wujcik*

9:25 Paper 287e: Point-of-Need Quantitative Detection of Trihalomethanes in Environmental Water Samples Using a Highly Sensitive and Selective Fiber-Based Preconcentration System — ***Hadi Rouhi***, *Colton Duprey, Nicole Penners, Emily Linn, Sarah Veres, George Chen, Ali Alshaikh, Yang Lu, Leigh Terry, Mark Elliott, Evan Wujcik*

9:40 Paper 287f: Electrochemical Detection of Cd(II) Using Nano-Electrodes in Environmental Samples — ***Muzammil Nishar Ahmed***, *Wendy Zhou, Pavithra Pathirathna*

9:55 Paper 287h: Facile Carbon Electrode Modification for Improved Biosensing — ***Gang Fan***

(288) Sustainable Pathways to Clean Hydrogen and Synthetic Fuels I

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, W-103B

William Gibbons, Chair
Eric Miller, Co-Chair

Sponsored by: Sustainable Pathways Toward Hydrogen and Synthetic Fuels

8:00 Paper 288a: Integration of Green Hydrogen Value Chains for Energy-Intensive Industries with Wider Energy Systems: Whole-Systems Modelling and Optimisation — ***Sheila Samsatli***, *Nouri John Samsatli*

8:25 Paper 288b: Safety and Security Analysis of a Potential Remote Offshore Green Hydrogen Production — *Ahmed Elkady, Faisal Khan, Mahmoud El-Halwagi,* ***Moustafa Ali***

8:50 Paper 288c: Modeling the Impact of Degradation on the Cost of Low-Temperature Electrolytic Hydrogen Production — ***Landon Schofield***, *Benjamin Paren, Doo Hyun Mark Chung, Yang Shao-Horn, Dharik Mallapragada*

9:15 Paper 288d: Solar Thermochemical Water Splitting Using Iron Aluminates — ***Kent J. Warren***, *Justin Tran, Alan Weimer*

9:40 Paper 288e: Crystal Features Controlling Oxygen Vacancy Formation in ABO_3 Perovskites — ***Robert Wexler***, *Gopalakrishnan Sai Gautam, Ellen B. Stechel, Emily Carter*

10:05 Paper 288f: Aldehydes Oxidation-Assisted H_2 Production at High Current Densities Promoted By a Cooperative Catalyst — *Yue Chen,* ***Yang Hou***

10:30: Break

(289) CO2 Capture, Utilization, and Disposal: Key to Clean Energy Production

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-227B

Ambalavanan Jayaraman, Chair
Burcu Gurkan, Co-Chair

Sponsored by: Transport and Energy Processes

8:00 Paper 289a: Multi-Scale Modeling of Novel Amine-Based Solvents for CO_2 Capture — ***Ismail Alkhatib***, *Daniel Bahamon, Lourdes Vega*

8:20 Paper 289b: Multi-Scale Dynamic Modeling and Techno-Economic Analysis of a Radial Flow Fixed Bed Contactor for Post-Combustion CO_2 Capture — ***Ana Flavia Monteiro***, *Ryan Hughes, Debangsu Bhattacharyya*

8:40 Paper 289c: Development of a Novel Cu-Based Dual Function Material for CO_2 Capture and Conversion — *Rim Ismail, Mohammed Ali Saleh,* ***Abdelbaki Benamor***, *Sardar Ali, Muftah El-Naas*

9:00 Paper 289d: High Surface Area Guanidine Based Sorbents for CO_2 Capture — ***Mani Modayil Korah***, *Matthew D. Green*

9:20: Break

9:40 Paper 289f: A Passive Wind Collector Integrated with a Direct Air Capture (DAC) System for Efficient, Sustainable, and Scalable CO_2 capture — ***James Akinjide***, *Joo-Youp Lee, Aashish Priye*

10:00 Paper 289g: Novel Facilitated Transport Membrane for Low Cost Carbon Capture in Cement, Steel, and Steam Methane Reforming — ***Christine Parrish***, *Ken Loprete, Sudip Majumdar*

(290) Andreas Acrivos Award for Professional Progress in Chemical Engineering Lecture

Tuesday, Nov 15, 11:15 AM
Phoenix Convention Center, North Ballroom 120D

David Schaffer, Chair

Sponsored by: Awards Committee

11:15 Paper : Building Microbial Chemical Factories: Design, Assembly, and Engineering of Biological Routes to Chemical Compounds — ***Kristala Prather***

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(291) Renewable Polymers and Intermediates Technology

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-221C

Melody Morris, Chair
Wui Yarn Daphne Chan, Co-Chair
Shaibal Roy, Co-Chair

Sponsored by: Process Research and Innovation

12:30 Paper 291a: Upcycling of Polypropylene through Thermal Pyrolysis Using Mechano-Chemical Methods — ***Amy Le***, *Ramanan Krishnamoorti*

12:55 Paper 291b: Strong, Ductile and Resilient Functionalized Degradable Poly(alpha-Hydroxy Acids) — ***Xiaoqian Wang***, *Rong Tong*

1:20 Paper 291c: Renewable Polymers Via Direct Functionalization of Lignocellulosic Sugars — ***Lorenz Manker***, *Graham Dick, Adrien Demongeot, Maxime Hedou, Christele Rayroud, Thibeault Rambert, Marie Jones, Irina Sulaeva, Mariella Vieli, Antje Potthast, François Maréchal, Veronique Michaud, Harm-Anton Klok, Jeremy Luterbacher*

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(292) Catalyst Design, Synthesis, and Characterization V: Novel Catalysts

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-127C

Abdoulaye Djire, Chair
Gina Noh, Co-Chair
Nathaniel Eagan, Co-Chair

Sponsored by: Catalysis

12:30 Paper 292a: Effect of CNT on the Catalytic Activity of Cs-Ru/CeO_2 catalyst in Microwave-Assisted Ammonia Synthesis — ***Alazar Araia***, *Yuxin Wang, Jianli Hu*

12:48 Paper 292b: Increased Accessibility in Gold Clusters Using Bis-Diphenyphosphine Ligands — *Sayed Abu Sufyan,* ***Michael Nigra***

1:06 Paper 292c: Tuning the Rate and Selectivity of Formic Acid Decomposition through Strong Metal Support Interaction Phenomena in Transition Metal Borides. — ***Tej Choksi***, *Luan Q. Le, Wen Liu, Renhong Li, Lavie Rekhi, Roong Jien Wong, Mingwu Tan, Hui Ling Tan*

1:24 Paper 292d: Controlling Catalysts' Structure and Methane Oxidation Performance Using Flame Spray Pyrolysis — ***Can Wang***, *Musa Najimu, Erdem Sasmaz*

1:42 Paper 292e: Reversible Ionic Liquids (RevILs) for the Preparation of Thermally Stable SBA-15 Supported Gold Nanoparticle Catalysts — ***Zengran Sun***, *Ellis Hammond-Pereira, Xianghui Zhang, Di Wu, Steven Saunders*

2:00 Paper 292f: Simple, Fast, and Scalable Atomically Controlled Synthesis of Heterogeneous Catalysts — ***Abolfazl Shakouri***, *Horie Adabi Firouzjaie, Stavros Karakalos, Christopher Williams, John Regalbuto*

2:18 Paper 292g: Supported Single Atom Catalyst Design, Synthesis, and Characterization Via Chelate Fixation Method — ***Brian Vakili***, *Shima Oruji, Abolfazl Shakouri, John Regalbuto, Christopher Williams*

2:36: Break

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(293) Catalytic Upcycling of Waste Plastics II: Focus on Commodity Plastic Waste and Beyond

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-128A

Hilal Ezgi Toraman, Chair
Tibor Szilvasi, Co-Chair
Wan-Ting Chen, Co-Chair

Sponsored by: Catalysis

12:30 Paper 293a: Polyolefin Upcycling over Earth-Abundant Catalysts — ***Brandon Vance***, *Pavel Kots, Cong Wang, Dionisios Vlachos*

12:48 Paper 293b: Investigation of the Effect of Commercial ZSM-5 Catalysts and Their Modified Forms in the Pyrolysis Reaction of Polyethylene. — ***Paola Arango Ponton***, *Guillaume Corjon, Sophie Duquesne, Jean-François Lamonier*

1:06 Paper 293c: Pathway to a Plastic Circular Economy: Intrinsic Kinetics of Polyethylene Pyrolysis Via Pulse-Heated Analysis of Solid Reactions (PHASR) — ***Isaac Mastalski***, *Nathan Sidhu, Paul Dauenhauer*

1:24 Paper 293d: Zeolite Supported Pt for Depolymerization of Low-Density Polyethylene By Induction Heating — ***Bernard Whajah***, *Joseph Heil, James Dorman, Kerry Dooley*

1:42 Paper 293e: Understanding and Avoiding Mass Transport Limitations to Enable Catalyst Design for Low Temperature Polyolefin Cleavage and up-Cycling — ***Max Mortensen Jr.***, *Siris Laursen*

2:00 Paper 293f: Screening Catalysts for Hydrothermal Recycling of Post-Consumer PET Waste — ***Patricia Pereira***, *Phillip E. Savage, Christian Pester*

2:18 Paper 293g: Upcycling Waste Polyurethane into Value-Added Chemicals By Sub-and Supercritical Water — ***Vahab Ghalandari***, *Toufiq Reza*

2:36 Paper 293h: Catalytic Dehydration of Evoh with Heterogeneous Acid Catalysts — ***Luis Trevisi***, *Lance Lobban, Steven Crossley, Bin Wang*

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(294) Fundamentals of Catalysis and Surface Science V: Electrocatalysis and photocatalysis

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-128B

Alyssa Hensley, Chair
Junjie Chen, Co-Chair

Sponsored by: Catalysis

12:30 Paper 294a: A Kinetic Analysis of the CO Electro-Oxidation Reaction on Bimetallics: Understanding the Interplay of Bifunctional and Electronic Effects — *Adam Baz,* ***Adam Holewinski***

12:52 Paper 294b: Fundamentals of Catalytic Surfaces with Charge Condensation — ***Paul Dauenhauer***

1:14 Paper 294c: Characterizing the Interplay between Molecular-Surface Interactions, Catalyst Reconstruction, and Performance: Hydrogen Oxidation over Pt-Based Bimetallic Catalysts — *Ayodeji Omoniyi,* ***Alyssa Hensley***

1:36 Paper 294d: Importing Hydroformylation Catalysts on Electrode Surfaces Unlocks Novel Voltage-Driven Reactivity — ***Joy Zeng***, *Karthish Manthiram*

1:58 Paper 294e: Conductive Alumina-Graphene Catalytic Condenser for Programmable Solid Acid — ***Tzia Ming Onn***, *Phillip Christopher, K. Andre Mkhoyan, Matthew Neurock, Omar Abdelrahman, C. Daniel Frisbie, Paul Dauenhauer*

2:20 Paper 294f: Pulsed Photon Illumination to Control Catalytic Chemistry at a Metal Nanoparticle Surfaces — ***Isabel Barraza Alvarez***, *Phillip Christopher*

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(295) In Honor of the 2020 R.H. Wilhelm Award Winner II (Invited Talks)

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-127A

Marc Porosoff, Chair
Daniel Esposito, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

12:30: Welcoming Remarks

12:35 Paper 295a: Modeling Ternary Alloy Segregation with Density Functional Theory and Machine Learning — *Yilin Yang, Zhitao Guo, Andrew J. Gellman,* ***John Kitchin***

12:56 Paper 295b: Transition Metal Nitride-Based Catalysts for Electrochemical Nitrogen Reduction and Hydrogen Evolution Reactions — ***Shyam Kattel***, *Damilola Ologunagba*

1:17 Paper 295c: How to Dress an Electrocatalyst — ***Daniel Esposito***

1:38 Paper 295d: Surface Sensitive Measurement Techniques for Enhanced Understanding of Electrocatalytic Processes — ***Brian Tackett***

1:59: Introductory Remarks

2:15 Paper 295e: Chemical Engineering Approaches for Catalytic Reduction of CO_2 — ***Jingguang G. Chen***

(296) In Honor of Vemuri Balakotaiah's Birthday (Invited Talks)

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-127B

David West, Chair
Michael Harold, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

12:30 Paper 296a: Autothermal Reactor Design for Oxidative Coupling of Methane — *Laurien A. Vandewalle, Kevin Van Geem,* ***Guy B. Marin***

12:55 Paper 296b: Multi-Scale Coarse-Graining of Diffusion-Convection-Reaction Models — ***Ram R. Ratnakar***

1:20 Paper 296c: Multiscale Modeling of Mixotrophic Algal Cultivation in Pilot-Scale Photobioreactors with Synergistic Integration of CO_2 Sequestration and Wastewater Treatment — ***Saikat Chakraborty****, Arun K. Mehta*

1:45 Paper 296d: Packed Bed Reactor Experiment: Operating a Two-Phase Reactor Bed in Space — ***Mahsa Taghavi****, Brian J. Motil*

2:10 Paper 296e: Spatiotemporal Features of Environmental Catalysts — ***Michael Harold***

2:35 Paper 296f: Some Examples of the Impact of Prof. Balakotaiah's Work in the Chemical Industry — ***David West***

(297) Spotlights in Thermodynamics and Computational Molecular Science (Invited Talks)

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-224AB

M. Scott Shell, Chair
Shikha Nangia, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

12:30 Paper 297a: Embedding Stereoelectronic Effects into Molecular Representations for Machine Learning — ***Gabriel dos Passos Gomes***

12:53 Paper 297b: Predicting Solubility Limits of Organic Solutes for a Wide Range of Solvents and Temperatures Using Machine Learning and Thermodynamics — ***Florence Vermeire****, Yunsie Chung, William Green*

1:16 Paper 297c: Towards a Universal Adsorption Model Using Machine Learning: Motivation, Progress and Challenges — ***Diego Gomez Gualdron***

1:39 Paper 297d: Atomistic Simulations of RNA Folding in Bulk Aqueous Solutions and under Confinement — ***Gul Zerze***

2:02 Paper 297e: Thermodynamic Stability of Multimetallic Nanoparticles — ***Giannis Mpourmpakis***

2:25 Paper 297f: Probing Realistic Water-2D Material Interfaces Via Combined Quantum and Classical Simulations — ***Ananth Govind Rajan***

(298) Advances in Computational Methods and Numerical Analysis - I

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, W-101A

Joel Paulson, Chair
Matthew Stuber, Co-Chair
Wheaton Schroeder, Co-Chair

Sponsored by: Applied Mathematics and Numerical Analysis

12:30 Paper 298a: Learning Continuous Models for Continuous Physics — ***Aditi Krishnapriyan***

12:49 Paper 298b: Enabling Interpolation of Sparse Data Via Neural ODEs — ***William Bradley****, Ron Volkovinsky, Fani Boukouvala*

1:08 Paper 298c: Quantifying the Invertibility of Neural Networks and Their Transformations — ***Tianqi Cui****, Thomas Bertalan, Ioannis G. Kevrekidis, Mahyar Fazlyab*

1:27 Paper 298d: Staying the Course: Locating Fixed Points of Dynamical Systems (and Critical Points of Potentials) on Riemannian Manifolds Defined By Sampling Point-Clouds — ***Anastasia Georgiou****, Juan Bello-Rivas, John Guckenheimer, Ioannis G. Kevrekidis*

1:46 Paper 298e: Manifold Learning Post-Processing Galerkin Algorithms for Dissipative PDEs on Their Approximate Inertial Manifolds — ***Cristina Martin Linares****, Thomas Bertalan, Nikolas Evangelou, Edriss S. Titi, Ioannis G. Kevrekidis*

2:05 Paper 298f: Application of Systems of Differential Algebraic Equations to Kinetic Models of Metabolism — ***Patrick Suthers****, Costas D. Maranas*

2:24 Paper 298g: Efficient Numerical Schemes for Population Balance Models — ***Pavan Inguva****, Kaylee C. Schickel, Richard D. Braatz*

2:43 Paper 298h: Perspectives on Quantum Computing for Chemical Engineering: A Joint View from Academia and Industry — ***David Bernal***

(299) Advances in Process Control II

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, W-101B

Daniel Rivera, Chair
Ravendra Singh, Co-Chair

Sponsored by: Systems and Process Control

12:30 Paper 299a: Stable Economic Nonlinear Model Predictive Control without a Pre-Calculated Steady-State Optimum — ***Kuan-Han Lin****, Lorenz Biegler*

12:49 Paper 299b: Hybrid Model-Based MPC with Guarantees on Stability and Applicability Domain: Application to Chemical, Biochemical, and Hydraulic Fracturing Systems — ***Mohammed Saad Faizan Bangi****, Joseph Kwon*

1:08 Paper 299c: Model Predictive Control As a Reinforcement Learning Policy: Faster Learning Via Policy Rollouts — ***Elijah Hedrick****, Katherine Hedrick, Debangsu Bhattacharyya, Stephen Zitney, Benjamin P. Omell*

1:27 Paper 299d: Model-Based Fault Diagnosis and Fault Tolerant Control for Safety-Critical Chemical Reactors — ***Pu Du****, Joshiba Ariamuthu Venkidasalapathy, Sunjeev Venkateswaran, Benjamin Wilhite, Costas Kravaris*

1:46 Paper 299e: Quantum Technologies and Model Predictive Control — ***Kip Nieman****, Helen Durand*

2:05 Paper 299f: Stability-Preserving Automatic Tuning of PID Control with Reinforcement Learning — *Ayub Lakhani,* ***Myisha Ahmed Chowdhury****, Qiugang Jay Lu*

2:24 Paper 299g: An Advanced MPC for Nonlinear Large-Scale Dynamic Systems Based on Data-Driven POD/ANNs Method — ***Weiguo Xie***

2:43 Paper 299h: Quantitative Comparison of Model-Free Reinforcement Learning and Data-Driven Model Based Optimal Control — ***Tae Hoon Oh***

(300) In Honor of Professor Rex Reklaitis' 80th Birthday (Invited Talks)

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, W-102A

Venkat Venkatasubramanian, Chair
Selen Cremaschi, Co-Chair

Sponsored by: Information Management and Intelligent Systems

12:30 Paper 300a: Introduction — ***Venkat Venkatasubramanian***

12:35 Paper 300b: Rex Reklaitis: Operations Research and Process Systems Engineering — ***Ignacio Grossmann***

12:52 Paper 300c: Process Systems Engineering Approaches for Integrated Process Operations — ***Marianthi Ierapetritou***

1:09 Paper 300d: Pharmaceutical Systems Engineering: Past, Present and Future — ***Zoltan Nagy***

1:26 Paper 300e: It's All about Timing! — ***Ioannis (Yannis) P. Androulakis***

1:43 Paper 300f: You Want to Do What? Rex's Brainchild: The New Directions Committee (1996 – 2006) — ***Deborah Grubbe***

2:00 Paper 300g: Honoring Prof. Reklaitis' Contributions to Mentoring and Energy and Sustainability Research — ***Bri-Mathias Hodge***

2:17 Paper 300h: Some Thoughts on the Future of Advanced Drug Delivery Systems: New Materials and Models — ***Nicholas Peppas***

2:34 Paper 300i: Navigating Scheduling Research through Professor Reklaitis' Career & Contributions — ***Efstratios N. Pistikopoulos***

2:51 Paper 300j: Concluding Remarks - — ***Selen Cremaschi***

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(301) Industrial Applications in Design and Operations

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, W-101C

Burcu Beykal, Chair
Maria Papathanasiou, Co-Chair

Sponsored by: Systems and Process Operations

12:30 Paper 301a: Addressing Practical Considerations in Implementation of Optimization Models for the Chemical Process Industry — ***Shachit S. Iyer***, *Sreekanth Rajagopalan, Scott J. Bury*

12:48 Paper 301b: Real-Time Optimization: Current Status & Opportunities — ***Dimitrios Georgis***, *John Righi*

1:06 Paper 301c: Estimation of Cost Savings By Co-Serving Customers in Vendor-Managed Inventory Distribution — ***Abilash Subbaraman***, *Zachary Wilson, Ayman Mhamdi, Mukesh Rungta, Jeffrey E. Arbogast, Chrysanthos Gounaris*

1:24 Paper 301d: Economic Evaluation of Infrastructures for Pyrolysis-Based Upcycling of Plastic Waste — ***Jiaze Ma***, *Philip Tominac, George Huber, Olumide Olafasakin, Mark Mba Wright, Victor Zavala*

1:42 Paper 301e: A Predictive Approximation Based on Squeeze Functional in Solving Large Scale Dynamic Simulation Problems — ***Gang Xu***

2:00 Paper 301f: Grid-Responsive Smart Automation Methods to Incorporate Renewable Energy Sources – a Case Study — ***Yunzhi Chen***, *Blake Billings, Sammy Partridge, Brittany Pruneau, Kody Powell*

2:18 Paper 301g: Bayesian Desirability Function Optimization of Cell Culture Media for Cellular Agriculture — ***Zachary Cosenza***, *David E. Block*

2:36 Paper 301h: Proad (Process Advisor): Health Monitoring Dashboards for Compressors and Insulations — *Phee Nai Soon, Priyanka Gurung,* ***Srikar Venkataraman Srinivas***, ***Iftekhar Karimi***, ***Farooq Shamsuzzaman***, *Rajagopalan Srinivasan, Lakshminarayanan S.*

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(302) Brown-bag Lunch-and-Learn: Teaching Tips

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, W-105B

Jennifer Pascal, Chair
Stephanie Velegol, Co-Chair

Sponsored by: Education

12:30: Break

12:45: Welcoming Remarks

12:50 Paper 302a: Constructing a Syllabus with an Accessible Community in Mind — ***Jeffrey Halpern***, *Mariah Arral*

1:00 Paper 302b: Recalibrating Student Learning Goals Using Bloom's Taxonomy — ***Christy West***

1:10 Paper 302c: Is Jango Fett's Backpack Thermodynamically Feasible? Bringing Students' Interest into Chemical Engineering Courses Using YouTube Problems — ***Matthew Liberatore***

1:20 Paper 302d: Improving Student Writing: Drafts & Reflections on Lab Reports — ***Katie Cadwell***

1:30 Paper 302e: Art Conservation and Chemical Engineering Product Design — ***Rebecca Harmon***

1:40 Paper 302f: Let's Talk about Process Safety: Utilizing an Online Forum-Based Approach to Discuss Process Safety Incidents — ***Richard Cimino***

1:50: Discussion

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(303) In Honor of the 2021 Recipient of the Warren K. Lewis Award - Nicholas Peppas - Part II (Invited Talks)

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, W-105A

Surya Mallapragada, Chair
Antonios Mikos, Co-Chair

Sponsored by: Education

12:30 Paper 303a: The People Who Get to Do the Science Determine What Science Gets Done: Elucidating the Impact of Red Blood Cell Rigidity in Sickle Cell Disease — ***Omolola Eniola-Adefeso***

1:00 Paper 303b: Entrepreneurial Bioengineering Research & Design Via Innovative Collaboration — ***Mark Byrne***

1:30 Paper 303c: The Role of Bioengineering in an Evolving Chemical Engineering Curriculum — ***Efrosini Kokkoli***

2:00 Paper 303d: Modern Bioengineering and Its Home in Chemical Engineering — ***Hal Alper***

2:30 Paper 303e: Inclusive and Equitable Teaching Methods in Chemical Engineering — ***Shelly Peyton***

3:00: Concluding remarks

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(304) Tuesday LGBTQ+ & Allies Safe Zone Workshop

Tuesday, Nov 15, 2:00 PM
Phoenix Convention Center, N-231B

Anthony Butterfield, Chair

Sponsored by: LGBTQ+ and Allies Community

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(305) Computational Studies of Early-Stage and Low-Dimensional Self-Assembly

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-223

Julia Dshemuchadse, Chair
Sumit Sharma, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

12:30 Paper 305a: Optimal Reaction Coordinates for Heterogeneous Nucleation of Densely Packed Atomic and Colloidal Crystals — *Tiago Domingues, Sarwar Hussain,* ***Amir Haji-Akbari***

12:45 Paper 305b: Topographical Defects Can Confer Exceptional Ice Nucleation Ability to Mediocre Nucleants — ***Yuqing Qiu***, *Atanu Metya, Valeria Molinero*

1:00 Paper 305c: Effect of Nonlinear Diffusion on Travelling Wave and Turing Patterns in Autocatalytic Systems — ***Uttam Kumar***, *Subramaniam Pushpavanam*

1:15 Paper 305d: Free Energy Contributions to Template-Assisted Self-Assembly of Sub-10 Nm Particles from Steered Molecular Dynamics Simulations — *Zhen Luo,* ***Shafigh Mehraeen***

1:30 Paper 305e: Image-Based State Representation of 2D Colloidal Self-Assembly Systems. — ***Andres Lizano***, *Xun Tang*

1:45 Paper 305f: Phase Behavior and Morphological Features of Self-Assembled Magnetic Handshake Panels — ***Andreia Fenley***, *Chrisy Xiyu Du, Ran Niu, Itai Cohen, Michael P. Brenner, Julia Dshemuchadse*

2:00 Paper 305j: Molecular features underlying phase separation of protein-nucleic acid condensates revealed by a new coarse-grained DNA model — ***Utkarsh Kapoor**, Jeetain Mittal*

2:15 Paper 305h: Thermodynamics and Kinetics of Biomolecular Condensation from Simulations and Experiments in Small, Finite Volumes. — *Lunna Li, Matteo Paloni, Umberto Capasso Palmiero, Paolo Arosio, Alessandro Barducci, **Matteo Salvalaglio***

2:30 Paper 305i: A Strong Nonequilibrium Bound for Sorting of Cross-Linkers on Growing Biopolymers — ***Yuqing Qiu**, Michael Nguyen, Glen M. Hocky, Aaron Dinner, Suriyanarayanan Vaikuntanathan*

(306) Connecting the Dots in Industry (Invited Talks)

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-232C

Christopher Wirth, Chair
Caroline Szczepanski, Co-Chair
Ning Wu, Co-Chair

Sponsored by: Interfacial Phenomena

12:30 Paper : Resolve Polyolefin Adhesion Challenge to High Performance Athletic Shoes and Outlook in Sustainability — ***Grace Wan**, Colin Li Pi Shan, Yongchun Chen, Brian Yu*

1:00 Paper : Soft Matter, Colloids, and Interfacial Phenomena Challenges in Small Molecule Pharmaceutical Product Development — ***Stephanie Lam***

1:30 Paper : Designing Polymers to Adhere to Surfaces — ***Ann Fornof***

(307) Electrochemical Fundamentals: Faculty Candidate Session I

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-232B

Wenzhen Li, Chair
Shuya Wei, Co-Chair

Sponsored by: Electrochemical Fundamentals

12:30 Paper 307a: Understanding and Controlling Pseudocapacitance in Electrochemical Energy Storage: Design of Fast Charging and Low-Temperature Hybrid Battery Systems — ***Theresa Schoetz**, Robert Messinger*

12:45 Paper 307b: Transient Batteries for Self-Powered Bioelectronics — ***Yamin Zhang**, John A. Rogers*

1:00 Paper 307c: Elevated Temperature Performance of the All-Aqueous Copper Thermally Regenerative Battery — ***Nicholas Cross**, Matthew Rau, Serguei Lvov, Christopher Gorski, Bruce E. Logan, Derek Hall*

1:15 Paper 307d: Engineering the Micro- and Atomic-Structures of Layered Cathode Materials Based on Oxidation States of Transition Metal Dopants — ***H. Hohyun Sun**, Un-Hyuck Kim, Adam Heller, C. Buddie Mullins*

1:30: Break

1:45 Paper 307e: Revealing the Dynamics of Solid-Electrolyte Interphase (SEI) at Li Metal Anode — ***Weilai Yu**, Zhenan Bao*

2:00 Paper 307f: Establishing Design Principles for Redox Flow Batteries with Suspension-Based Electrolytes — ***Madhu Venkata Rama Krishna Majji**, James Swan, Fikile R. Brushett*

2:15 Paper 307g: Rational Design of Atomically Dispersed Single Atom Catalysts for Electrochemical Reactions — ***Md Delowar Hossain***

2:30 Paper 307h: Interfacing Electrochemical and Biological Processes Enables Efficient Bioproducts Synthesis from Carbon Dioxide — ***Peng Zhang**, Susie Dai, Joshua Yuan*

2:45 Paper 307i: Kinetic and Thermodynamic Aspects of Voltage As a Driving Force for Ammonia Activation — ***Zachary Schiffer**, Karthish Manthiram*

(308) Fundamental Research in Transport Processes

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-230

Samaneh Farokhirad, Chair
Joel Plawsky, Co-Chair

Sponsored by: Transport Processes

12:30 Paper 308a: A Unified Theory of Free Energy Functionals and Applications to Diffusion — *Andrew Li, Leonid Miroshnik, Brian Rummel, Ganesh Balakrishnan, Sang Han, **Talid Sinno***

12:48 Paper 308b: Natural Convection Effects in Insulation Systems of Large-Scale Cryogenic Storage Tanks — ***Mahsa Taghavi**, **Swapnil Sharma**, Ram R. Ratnakar, Vemuri Balakotaiah*

1:06 Paper 308c: Flow in Porous Media: Similarity between the Velocity Magnitude and the Pore-Volume Distributions — ***Vi Nguyen**, Ngoc Hong Pham, Dimitrios Papavassiliou*

1:24: Break

1:42 Paper 308e: Geometrical Abstraction Using Mazes to Guide Rational Design of Engineered Systems — *Alex Guo, William Marshall, Corey Woodcock, **Joel Plawsky***

2:00 Paper 308f: High-Viscosity Cavitating Flow-through Vortex-Based Hydrodynamic Cavitation Device: Pressure Drop, Inception and Flow Characteristics — *Abhijeet Thaker, Ketan Madane, **Vivek V. Ranade***

2:18 Paper 308g: Shallow Water Analysis and Numerical Simulation of Laminar Planar Hydraulic Jump in Bingham Plastic Flow through an Open Rectangular Channel — *Banashree Samanta, **Gargi Das**, Subhabrata Ray, Manish Kaushal*

2:36 Paper 699i: Modeling Solvent Absorption in Highly Cross-Linked Polymer Resins with PC-SAFT — *Stefan Wagner, Patrick Krenn, Roland Nagl, Michael Fischlschweiger, **Tim Zeiner***

(309) Honorary sessions for Keith Gubbins' 85th birthday

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-222B

Erik Santiso, Chair
Kaihang Shi, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

12:30 Paper 309a: Carbon Nanostructure-Mediated Ultra-Rapid Separation — ***Katsumi Kaneko***

12:48 Paper 309b: The Enduring Legacy of Molecular Simulation and of Keith Gubbins — ***Paulette Clancy***

1:06 Paper 309c: Molecular Understanding, Design and Development of Ultralow Fouling Zwitterionic Materials — ***Shaoyi Jiang***

1:24 Paper 309d: Structures of Ice Confined in Nanopores; Pressure Enhancement and Wetting Energy Effects — ***Malgorzata Sliwinska-Bartkowiak***

1:42 Paper 309e: Computational Studies Reveal Varied Mechanisms of Oncogenic Activation amidst a Varied Mutational Landscape in Cancer Patients — *Keshav Patil, Krishna Suresh, Yiming Wang, Mark A. Lemmon, Yael Mosse, **Ravi Radhakrishnan***

2:00 Paper 309f: Emergence of Spontaneous Order in the Dynamics of Birds Flocking: A Statistical Teleodynamics Perspective — *Abhishek Sivaram, **Venkat Venkatasubramanian***

2:18 Paper 309g: Monte Carlo and Molecular Dynamics Study of Zeolite-Templated Carbon-Based Membranes for Hydrogen Purification from Steam Methane Reforming — ***Lourdes Vega**, Daniel Bahamon, Maryam Khaleel, Eun Seon Cho*

2:36 Paper 309h: Quantifying Confinement Effects on Fluid Transport Via Multi-Scale Simulations — ***Alberto Striolo***

(310) Particulate and Multiphase Flows: Emulsions, Bubbles, Droplets

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-231C

Reza Foudazi, Co-Chair
Vivek Sharma, Co-Chair

Sponsored by: Fluid Mechanics

12:30 Paper 310a: Rheology of Concentrated Nanoemulsions — *Zahra Abbasian Chaleshtari,* ***Reza Foudazi***

12:45 Paper 310b: Controlling the Nonlinear Rheology of Emulsions Using Telechelic Block Copolymers — *Daniel Keane,* ***Ryan Poling Skutvik***

1:00 Paper 310c: Numerical Investigation of the Role of Surface Viscosity on Droplet Breakup and Relaxation in Extensional Flow — ***Natasha Singh****, Vivek Narsimhan*

1:15 Paper 310d: High Throughput Measurement of Droplet Surface Tension in Confined Flows — *Evyatar Shaulsky,* ***Sara Hashmi***

1:30 Paper 310e: Effect of Critical Geometric and Physical Parameters on the Coalescence Dynamics of Droplet Pairs in Confined Shear Flows — ***S M Abdullah Al Mamun****, Samaneh Farokhirad*

1:45 Paper 310f: Turbulent Droplet Breakage in a Von Kármán Flow Cell — ***Krishnamurthy Ravichandar****, R. Dennis Vigil, Rodney Fox, Michael G. Olsen*

2:00: Break

2:15 Paper 310h: Fully 3D Magnetic Resonance Imaging of Bubble Dynamics in Viscous Dense Suspensions — *Wasif Zia, Alireza Bordbar, Janine Birnbaum, Boyuan Chen, Einat Lev,* ***Chris Boyce***

2:30 Paper 310i: Periodically Structured Coalescence of Bubbles in a Vertical Stream Rising through Dense Suspensions — ***Boyuan Chen****, Azin Padash, Wasif Zia, Alireza Bordbar, Javad Omidi, Chris Boyce*

(311) Rheology of Biomaterials and Biological Systems

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-232A

Danielle Mai, Co-Chair
Amanda Marciel, Co-Chair

Sponsored by: Fluid Mechanics

12:30 Paper 311a: Colloidal Model Applied to Viscosity of Dilute to Semi-Dilute Protein Suspensions — *Sabitoj Singh Virk,* ***Patrick Underhill***

12:45 Paper 311b: Electrospinning of End-Capped Oligopeptides — ***Prerana Rathore****, Brian Montz, Brittany Nelson, Stephen Nonnenmann, Todd Emrick, Jessica Schiffman*

1:00 Paper 311c: Manipulation of Coacervate Droplets with an Electric Field — ***Aman Agrawal****, Matthew V. Tirrell, Jack F. Douglas, Alamgir Karim*

1:15 Paper 311d: Influence of Counterion Solvation on the Properties of Polyelectrolytes and It's Application in Hand Sanitisers — ***Carlos Lopez***

1:30 Paper 311e: Predicting and Engineering Multiphase Behavior in Complex and Living Fluids — ***Krishna Shrinivas****, Michael P. Brenner*

1:45 Paper 311f: Cell Distributions and Segregation during Blood Flow in Sickle Cell Disease and Iron Deficiency Anemia within Straight and Serpentine Vascular Geometries — ***Xiaopo Cheng****, Christina Caruso, Wilbur A. Lam, Michael D. Graham*

2:00 Paper 311g: The Influence of Channel Curvature on Targeted Particle Binding in Macroscopic Blood Flow — ***Logan Piegols****, Omolola Eniola-Adefeso*

2:15 Paper 311h: *In-Situ* Magnetic Microrheology of Airway Mucus — ***Margaret Braunreuther****, Gerald Fuller*

2:30 Paper 311i: A Swimming Bacterium in a Two-Fluid Model of a Polymer Solution — ***Sabarish Vadanakurussi Narayanan****, Donald L. Koch, Sarah Hormozi*

2:45 Paper 311j: Interfacial Dynamics of Entangled Living Active Matter Collectives — ***Harry Tuazon****, Emily Kaufman, Daniel Goldman, M. Saad Bhamla*

(312) Fundamentals and Applications for Waste Treatment and Valorization

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-225A

Hyun-Tae Hwang, Chair
Heriberto Cabezas, Co-Chair
Yinlun Huang, Co-Chair
Robert Peters, Co-Chair

Sponsored by: Fundamentals

12:30 Paper 312a: Bioproducts from High-Strength Wastewater with the Carboxylate Platform Via Methane-Arrested Anaerobic Digestion — ***Haoran Wu****, Meltem Urgun-Demirtas, Mark Holtzapple, Phuong Thai, Rachel Dalke, Lauren Valentino*

12:48 Paper 312b: Self-Assembled Living Hydrogel for Valuable Metal Recovery from Electronic Waste — ***Le You****, Huan Hsuan Hsu*

1:06 Paper 312c: Engineering a New Self-Regenerative System to Achieve Effective Removal of Heavy Metal Contaminants from Polluted Waters — ***Sweta Roy****, Zehui Han, Dacheng Ren*

1:24 Paper 312d: Lipase Immobilization on Mesoporous Carbon and Evaluation As Catalysts in the Hydrolysis of Waste Oleochemical Streams — ***Alexander Baena****, Alvaro Orjuela*

1:42 Paper 312e: Valorization of Water Treatment Plant Residuals in the Production of a Biodegradable Deicer — ***Alexander Mathews***

2:00 Paper 312f: Fed-Batch Screening of Methanotroph-Algae Cocultures on Anaerobic Digester Effluent for Larger-Scale Wastewater Treatment and Valorization — ***Loyal Murphy****, Kiumars Badr, Riley O'Gwynn, Q. Peter He, Jin Wang*

2:18 Paper 312g: Recycling PVC Containing Wood Wastes for Value-Added Products — ***Xianglan Bai****, Xiaolin Chen*

2:36 Paper 312h: One-Pot Conversion of PVC Containing Co-Mingled Wastes — ***Xianglan Bai****, Xiaolin Chen*

(313) Remediation of Emerging Contaminants and Legacy Compounds

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-225B

Alexander Dowling, Chair
Sage Hiibel, Co-Chair
Robert Peters, Co-Chair

Sponsored by: Water

12:30 Paper 313a: Synthesis, Transport Properties, and Benefits of Multifunctional Membrane Platforms for the Separation of Contaminants from Aqueous Environments — ***Francisco Leniz****, Hailey Craft, Lindell Ormsbee, Dibakar Bhattacharyya*

12:55 Paper 313b: Pfas Degradation By a Thin Film Gas-Liquid Non Thermal Plasma Reactor — ***Narasamma Nippatlapalli****, Rachel Gallan, Radha Krishna Murthy Bulusu, Robert Wandell, Bruce R. Locke*

1:20 Paper 313c: Pfas Surfactant Sequestration By Binding to Functional Polymers — ***Paschalis Alexandridis****, Samhitha Kancharla, Aditya Choudhary, Dengpan Dong, Dmitry Bedrov, Marina Tsianou*

1:45 Paper 313d: Pfas Fate and Transport Study in Contaminated Sediments Utilizing Capping Methods and Sorbent Amendments — *Prashik Manwatkar,* ***Hossein Dallalzadeh Atoufi****, David Lampert*

2:10 Paper 313e: Superfine Activated Carbon-Functionalized Adsorptive Thin-Film Nanocomposite Membranes for Enhanced Pfas Removal from Water — ***Medha Kasula****, Milad Esfahani*

(314) Computational, Structure, Biophysical Protein Engineering

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-125A

Daniel Woldring, Chair
Robert Pantazes, Co-Chair

Sponsored by: Bioengineering

12:30 Paper 314a: Beginning with the End in Mind: Integrating Cell-Free Protein Synthesis with Coarse-Grained Simulation for Site-Specific Optimization of Protein Therapeutic Pegylation. — ***Brad Bundy***, *Emily Zhao, Mehran Soltani, Addison K. Smith, J Porter Hunt, Joshua W. Wilkerson, Thomas Knotts IV*

12:48 Paper 314b: Structural Characterization of an Effector-Biasing Interleukin-2 Immunocytokine — ***Joseph Gould***, *Elissa Leonard, Jamie Spangler*

1:06 Paper 314c: Novel Experimental and Computational Approaches for Conformational Antibody Engineering — ***Matthew Smith***, *Alec Desai, Jennifer Zupancic, Peter Tessier*

1:24 Paper 314d: Antibody Affinity and Specificity Co-Optimization Via Machine Learning — ***Patrick Kinnunen***, *Emily K. Makowski, Lina Wu, Jie Huang, Jennifer J. Linderman, Peter M. Tessier*

1:42 Paper 314e: Combining Protein Sequence and Structure Pretraining — *Hugh Yeh,* ***Kevin Yang***

2:00 Paper 314f: Computational Modeling of Sars-Cov-2 Spike RBD Binding to Human ACE2 Receptor Using Molecular Simulations and Machine Learning — ***Veda Sheersh Boorla***, *Chen Chen, Ratul Chowdhury, Deepro Banerjee, Victoria S Cavener, Ruth H Nissly, Abhinay Gontu, Nina R Boyle, Shubhada K Chothe, Lindsey LaBella, Padmaja Jakka, Santhamani Ramasamy, Kurt J Vandegrift, Meera Surendran Nair, Suresh V Kuchipudi, Costas D. Maranas*

2:18 Paper 314g: Exploring the Features of Protein-Protein Interfaces to Enable Protein Design for Chemical Engineering — ***Robert Pantazes***

(315) Drug Delivery

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-126A

Jessica Larsen, Chair
Handan Acar, Co-Chair
Whitney Stoppel, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

12:30 Paper 315a: Endoplasmic Reticulum (ER) Stress Decreases the Efficacy of Delivered siRNA Via Cholesterol Dysregulation — ***Ryan Splichal***, *Christina Chan, S. Patrick Walton*

12:48 Paper 315b: Anionic Bioconjugation Enables Intracellular Protein Delivery with Ionizable Lipid Nanoparticles — ***Azmain Alamgir***, *Matthew DeLisa, Christopher Alabi*

1:06 Paper 315c: Wireless Iontophoresis Lens Mediated Ocular Drug Delivery — ***Andrea Zuccaro***, *Sabrina Coffman, Naomi Addai Asante, Nicolas Hamouche, Donald S. Sakaguchi, Surya Mallapragada, Metin Uz*

1:24 Paper 315d: Formulation and Scale-up of Fast-Dissolving Lumefantrine Nanoparticles for Oral Malaria Therapy — ***Madeleine Armstrong***, *Leon Z. Wang, Kurt Ristroph, Chang Tian, Jiankai Yang, Lirong Ma, Shuhong Jiang, Santipharp Panmai, Donglu Zhang, Karthik Nagapudi, Robert K. Prud'homme*

1:42 Paper 315e: Oral Delivery of High Isoelectric Point Therapeutic Proteins Using pH-Responsive Nanoscale Complexation Hydrogels — ***Fabiola Chapa Villarreal***, *Heidi Oldenkamp, Avha Mohanty, Alex Chiu, Nicholas Peppas*

2:00 Paper 315f: Evaluation of Vegetarian Softgels Using SeaGel® Technology for Pharmaceutical Applications — ***Jin Zhao***, *Becca Putans, Benjamin Roscoe, Michael Evangelista, Thomas Watson, Teegan Penkala, Ian Gillespie, Dean Lee, Koudi Zhu, Michael Baumann*

2:18 Paper 315g: Invited Talk: Placeholder for the Drug Delivery Session — ***Whitney Stoppel***, *Jessica Larsen, Handan Acar*

(316) Food, Pharmaceutical & Bioengineering Faculty Candidates Session II

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-125B

Thomas J. Mansell, Chair
Adam Melvin, Co-Chair
Ryan Summers, Co-Chair
Mark Blenner, Co-Chair
Whitney Stoppel, Co-Chair
Maobing Tu, Co-Chair

Sponsored by: Food, Pharmaceutical & Bioengineering Division

12:30: Break

12:48 Paper 316b: N-Terminal Engineering Improves the Quality of Recombinant Proteins Secreted from Yeast — ***Neil C. Dalvie***, *Christopher Naranjo, Sergio Rodriguez Aponte, Ryan Johnston, J. Christopher Love*

1:06 Paper 316c: Antioxidant-Immobilized Backpack-Carrying Monocytes for TBI Therapy — ***Rick Liao***, *Samir Mitragotri*

1:24 Paper 316d: A Genetic Toolkit for Anaerobic Gut Fungi — ***Tejas Navaratna***, *Michelle O'Malley*

1:42 Paper 316e: Efflux of Cerebrospinal Fluid through Cervical Lymph Vessels Is Reduced in Aged Mice — ***Aditya Raghunandan***, *Ting Du, Maiken Nedergaard, Douglas Kelley*

2:00 Paper 316f: Self-Powered, Programmable, and Bioresorbable Drug Delivery Devices — ***Yamin Zhang***, *John A. Rogers*

2:18 Paper 316g: Engineering Functional Vascularization By Synthetic Regulation of Paracrine Signaling — ***Mai T. Ngo***, *Ahmad S. Khalil, Christopher S. Chen*

(317) Stem Cells and Tissue Engineering

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-126B

Laurel Hind, Chair
Whitney Stoppel, Co-Chair
Panagiotis Mistriotis, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

12:30 Paper 317a: Lactate Inhibits the Growth of Human Pluripotent Stem Cells without Affecting Pluripotency — ***Demetrios Stoukides***, *Emmanuel Tzanakakis*

12:48 Paper 317b: Skin Tissue Derived Neural Crest Stem Cells and Metabolic Requirements for Multipotency — ***Pihu Mehrotra***, *Izuagie Ikhapoh, Pedro Lei, Georgios Tseropoulos, Yali Zhang, Jianmin Wang, Song Liu, Stelios Andreadis*

1:06 Paper 317c: Impact of Oncostatin M & Tumor Necrosis Factor-α on Chondrogenic and Immunosuppressive Capacity of Human Mesenchymal Stem Cells in Pellet Culture and 3D Hydrogel Constructs — ***Carly Battistoni***, *Qinghua Xu, Rithika Athreya, Alyssa Panitch, Julie C. Liu*

1:24 Paper 317d: Surface Engineering of Auxetic Scaffolds for Neural and Vascular Differentiation from Human Stem Cells — ***Xingchi Chen***, *Chang Liu, Xiaolin Wang, Tristan Driscoll, Changchun Zeng, Yan Li*

1:42 Paper 317e: A Streamlined Protocol for Highly-Efficient Reprogramming to Induced Motor Neurons — ***Nathan Wang***, *Brittany Lende, Kate E Galloway*

2:00 Paper 317f: Light-Controlled Enhancement of Glucose-Stimulated Insulin Secretion of Optogenetically Engineered Human Pancreatic Beta-Cells — ***Zijing Chen***, *Emmanuel Tzanakakis*

2:18 Paper 317g: Invited Talk: Placeholder for Invited Talk for the Stem Cells and Tissue Engineering Session — ***Whitney Stoppel***, *Panagiotis Mistriotis, Laurel Hind*

(318) Advanced Separations Processes in Bioprocessing and Biomaterials

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-227C

Bandaru V. Ramarao, Chair
Sridharan Ramaswamy, Co-Chair

Sponsored by: Forest and Plant Bioproducts Division

12:30 Paper 318a: Robust Separation Process for Producing Pure Glucaric Acid Crystals from Fermentation Broth — ***Hoon Choi***, *Nathan Soland, Bonnie L. Buss, Stefan Haugen, Joel Miscall, Eric Tan, Eric Karp*

12:45 Paper 318b: Empowering Carbon Negative Bio-Chemicals with Advanced Electrochemical Separations — *Marcel Gausmann,* ***Christian Schröder****, Andreas Jupke*

1:00 Paper 318c: Microcrystalline Cellulose from Soybean Hull As an Excipient for Solid Dosage Forms: Powder Characterization and Tableting Properties — ***Navid Etebari Alamdari****, Burak Aksoy, Zhihua Jiang, Jayachandra B. Ramapuram*

1:15 Paper 318d: Numerical Analysis of Conventional Drying of Paper and Board — *Xinyi Li, Huajiang Huang,* ***Sridharan Ramaswamy***

(319) Fuel Processing for Hydrogen Production

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, W-103A

Dushyant Shekhawat, Chair
Daniel Haynes, Co-Chair

Sponsored by: Fuels and Petrochemicals Division

12:30 Paper 319a: Hydrogen Generation from Natural Gas Using Autothermal Chemical Looping Systems: Process Simulation and Heat Integration of Two Process Configurations — *Fanhe Kong, Yitao Zhang,* ***Pinak Mohapatra****, Andrew Tong, Liang-Shih Fan*

12:46 Paper 319b: Catalytic Conversion of Methane to Hydrogen and Carbon Nanotubes By Microwave Irradiation — ***Changle Jiang****, Brandon Robinson, Sonit Balyan, Jianli Hu*

1:02 Paper 319c: Exploring Production Aspects of Blue Hydrogen and Valuable CNTs from Natural Gas in a Fluidized Bed Reactor — ***Kaushal Parmar****, Kamal Pant, Shantanu Roy*

1:19 Paper 319d: Compact Flex-Fuel Processors for Syngas and Hydrogen Production — ***Hani Hawa****, Saurabh A. Vilekar, Christian Junaedi, Subir Roychoudhury*

1:36 Paper 319e: Ni-MgO Based NOVEL Catalysts Prepared By Combustion Synthesisfor CO_2 and Methane Reforming — *Vardan Danghyan, Alexander Mukasyan, Anand Kumar,* ***Eduardo E. Wolf***

1:53 Paper 319f: Solution Combustion Synthesis of Iron-Based Alumina Nanocomposites for Microwave-Assisted Thermocatalytic Dehydrogenation of Fossil Fuels — ***Zachary Chanoi****, Victoria Reyes, Evgeny Shafirovich*

2:10 Paper 319g: Use of the Ni-Ugso Catalyst for the Reforming of Methane Under Various Regimes and Industrial Hydrogen Production Conditions — ***Nicolas Abatzoglou****, Muhammad Irfan Malik, Esma Ines Achouri*

2:27 Paper 319h: Exploring the Potential of Ni_3S_2 Based Sulfur Looping Process for Efficient Production of H_2 from H_2s: A Thermodynamic and Kinetic Study — ***Anuj Joshi****, Kalyani Jangam, Zain Mohammad, Liang-Shih Fan*

2:43 Paper 319i: Integrated SOLID OXIDE Electrolytic Cell for a NOVEL Hydrogen Production Using Water-Energy Nexus Framework — ***Lateef Jolaoso****, Javad Asadi, Pejman Kazempoor*

(320) Breakthroughs in Sustainable Chemical Production and Process

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-228B

Zhongmin Liu, Chair
Emily Cole, Co-Chair
Mao Ye, Co-Chair

Sponsored by: Green Process and Product Engineering

12:30 Paper 320a: Automated, Multi-Task Bayesian Optimization of Pharmaceutical Processes — ***Connor Taylor***

1:00 Paper 320b: Chemical Looping Hydrogenation with Metal Oxide Bronzes for Selective Hydrogen Activation and Utilization — *Yifan Deng,* ***Evan Miu****, Giannis Mpourmpakis, James R. McKone, Goetz Veser*

1:30 Paper 320c: General Techno-Economic Analysis of Electrochemical Ammonia Production Processes with Various Nitrogen Sources — ***Juyeon Kim****, Woong Choi, Suhyun Lee, Jonggeol Na, Yun Jeong Hwang*

2:00 Paper 320d: Fractionation of Lignocellulosic Components By Environmental Benign Solvents — ***Zhimin Xue***

2:30 Paper 320e: Construction of an Enzymatic Shuttling Compartment Based on Reverse Micellar for Bamboo Biomass Hydrolysis in Ionic Liquids — ***Dan Wang****, Zhao Qin*

(321) Three Minute Thesis (3MT®) Competition

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-231A

Victoria Muir, Chair
Shelby Mills, Co-Chair
Hashim Al Hajji, Co-Chair
Hanaa Baniowda, Co-Chair
Cory Thomas, Co-Chair

Sponsored by: Young Professionals Committee (YPC)

(322) Plenary Session: Turbulence and Mixing – In Memory of Professor Robert Brodkey I (Invited Talks)

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-222C

Umit Ozkan, Co-Chair
James Hill, Co-Chair

Sponsored by: Miscellaneous

12:30: Introduction: Umit Ozkan, Ohio State University

12:40 Paper 322b: Bits and Pieces of the Turbulence Puzzle: A new length scale, deep structural similarity and a mechanism underlying diverse drag reduction strategies. — ***Ronald Adrian***

1:05 Paper 322c: Conditional Moment Methods for Turbulent Reacting Flows — ***Rodney Fox****, Aziz D. Ilgun, Alberto Passalacqua*

1:30 Paper 322d: Turbulent Velocity and Deformation Fields in Practical Dispersion Devices: Building on what Bob has taught us. — ***Richard Calabrese***

1:55 Paper 322e: Bob Brodkey: A Pioneer, A Super-Mentor, and A Passionate Explorer — ***Suzanne Kresta***

2:20 Paper 322f: Mixing and Packing of Binary Particles — ***Robert Pfeffer***

2:40 Paper 322g: Dr. Bob Brodkey - Teacher, Researcher and Visionary — ***Kris Lakshmanan***

3:00: Conclusion: James Hill, Iowa State University

(323) Leadership and Management of Sustainable Solutions in Industry

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, W-102B

Gayle Gibson, Chair
Raj Joshi, Co-Chair

Sponsored by: Management Division

(324) Area Plenary: Emerging Areas in Polymer Science and Engineering II (Invited Talks)

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-121B

Shudipto K. Dishari, Chair
Michelle Calabrese, Co-Chair
Siamak Nejati, Co-Chair

Sponsored by: Polymers

12:30 Paper 324a: Polymer Design in the Era of Automated Simulation and Experimentation — ***Juan De Pablo***

1:00 Paper 324b: Ion-Exchange Membranes with Ultrahigh Charge Densities — *David Kitto,* ***Jovan Kamcev***

1:30 Paper 324c: Solid State Electrolytes for Energy-Dense Lithium Metal Batteries — ***Chibueze Amanchukwu***

2:00 Paper 324d: Ionic Liquids Functionalized, Polymerized, and Encapsulated for CO2 Capture from Cabin Air and the Atmopshere — ***Burcu Gurkan***

2:30 Paper 324e: Exploring Single Polymer Conformation and Dynamics Using Single-Molecule Optical Microscopy — ***Muzhou Wang***

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(325) Biomaterial Scaffolds for Tissue Engineering II

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-122B

Amol Janorkar, Chair
Mario Moisés Álvarez, Co-Chair
Metin Uz, Co-Chair
Gulden Camci-Unal, Co-Chair

Sponsored by: Biomaterials

12:30 Paper 325a: Engineering Advanced Scaffolds for Tissue Engineering — ***Metin Uz***

12:48 Paper 325b: Ultraviolet-Assisted Direct Ink Writing of Pelvic Organ Prolapse (POP) Tissue Scaffolds — ***Yuxiang Zhu****, Kenan Song*

1:06 Paper 325c: One-Step Fabrication of Multi-Channel Hydrogel Scaffolds Using Chaotic Advection: Bioprinting of Pre-Vascularized Muscle-like Tissues — *Edna Johana Bolívar-Monsalve, Carlos Ceballos, Carolina Chavez Madero, Ali Khademhosseini, Paul S. Weiss, Mohamadmahdi Samandari, Ali Tamayol, Mario Alvarez,* ***Grissel Trujillo de Santiago***

1:24 Paper 325d: 3D Bioprinting of Regenerative, Corneal Cell-Laden Inks to Treat Corneal Blindness — ***Lucia G. Brunel****, Sarah M. Hull, Patrik K. Johansson, David Myung, Sarah C. Heilshorn*

1:42 Paper 325e: Adjusting Key Mechanical Properties of Lyophilized Silk Sponges to Determine the Effect on Enzymatic Degradation Rates — ***Henry Lutz****, Julie F. Jameson, Whitney Stoppel*

2:00 Paper 325f: Synthesis and Evaluation of Zwitterionic Peptide-Based Cross-Linkers for Nonfouling Hydrogel Applications — *Moubani Chakraborty, Adrienne Shea, Stephanie Haag, Kristopher V. Waynant,* ***Matthew Bernards***

2:18 Paper 325g: Improved Nerve Guide Conduit with Heparin-Collagen Layer-By-Layer Coatings Increase Adherence, Viability, and Protein Expression in Human Schwann Cells. — ***Luis Carlos Pinzon-Herrera****, Jorge Almodovar*

2:36 Paper 325h: Matrix Stiffness Regulates Proteome Profiling of Primary Hepatocytes and Extracellular Vesicles Secretion upon Alcohol Exposure and HIV Infection — ***Youra Moeun****, Raghubendra Singh Dagur, Murali Ganesan, Larisa I. Poluektova, Natalia A. Osna, Srivatsan Kidambi*

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(326) Biomimetic Materials I

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-121C

Xi Chen, Chair
Bret Ulery, Co-Chair
Yifan Cheng, Co-Chair
Christina Bailey-Hytholt, Co-Chair

Sponsored by: Biomaterials

12:30 Paper 326a: Biomimitic Hydrogels for Retinal Engineering — *Peng Zhao, Ronak Ansaripour, Sidi A Bencherif, Victor Hernandez-Gordillo, Linda G. Griffith, Michael Young, Petr Baranov, Deepti Singh,* ***Rebecca L. Carrier***

1:06 Paper 326b: Dynamic Recombinant Hydrogels with Degradation-Independent Relaxation Kinetics — ***Renato Navarro****, Michelle Huang, Julien G. Roth, Kelsea Hubka, Narelli Paiva, Sarah Heilshorn*

1:24 Paper 326c: Organic-Inorganic Interactions in 3D Printed Bouligand Nanostructures — ***Mohsen Esmaeili****, Kyle George, Nasser Nikfarjam, Nader Taheri-Qazvini, Monirosadat Sadati*

1:42 Paper 326d: Mimicking Biopolymer Structure in Synthetic Hydrogels for Model Extracellular Matrices — ***Logan D. Morton****, David A. Castilla-Casadiego, Ajay C. Palmer, Adrianne Rosales*

2:00 Paper 326e: Building the Bridge between Design and Function of Peptide-Based Materials — *Seren Hamsici, Gokhan Gunay,* ***Handan Acar***

2:18 Paper 326f: Exploration of Tertiary Structure in Sequence-Defined Polymers Using Molecular Dynamics Simulations — ***Kaylyn Torkelson****, Jim Pfaendtner*

2:36 Paper 326g: Designing Heterochiral Coiled Coils for Enhanced Binding and Enzymatic Stability in Biomaterials — ***Vincent Gray****, Rachel Letteri*

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(327) Electronic and Photonic Materials: Graduate Student Awards

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-121A

Matthew Crane, Chair
Elizabeth Lee, Co-Chair

Sponsored by: Electronics and Photonics

12:30 Paper 327a: Reversible Halogen Off-Gassing from Halide Perovskites: Connecting Point Defect Chemistry, Electronic Self-Doping, and Structural Disorder — ***Julian Vigil****, Nathan Wolf, Adam Slavney, Nicholas Weadock, Michael F. Toney, Hemamala Karunadasa*

12:43 Paper 327b: Thermoelectric Performance of Two-Dimensional Halide Perovskites Featuring Conjugated Ligands — ***Sheng-Ning Hsu****, Bryan Boudouris, Letian Dou*

12:56 Paper 327c: Lateral Growth of Lithium Enabled By Thin Film Electrical Resistance — ***Solomon Oyakhire****, Wenbo Zhang, Yi Cui, Stacey Bent*

1:09 Paper 327d: Chain Length Dependent Electron Transport Properties of Rigid-Rod Semiconducting Ladder Polymer — ***Duyen Tran****, Sarah West, Samson A. Jenekhe*

1:22 Paper 327e: Spectroscopic Characterization of Excitons in Two-Dimensional Semiconductors and Their Heterostructures — ***Zhen Lian****, Dongxue Chen, Xiong Huang, Yong-Tao Cui, Sufei Shi*

1:35 Paper 327f: Control of Thermal Transport at Ultrahigh Temperatures By Immiscible Oxide Heterostructures — ***Sean McSherry****, Matthew Webb, Jonathan Kaufman, Zihao Deng, Ali Davoodabadi, Tao Ma, Emmanouil Kioupakis, Keivan Esfarjani, John Heron, Andrej Lenert*

1:48 Paper 327g: The Profound Impact of Transient Heat Transfer on the Photovoltaic Properties of Solution-Processed Cu(In,Ga)Se_2 — ***Kyle Weideman****, Rakesh Agrawal*

2:01 Paper 327h: Tuning Optical Parameters of Nanocrystal-Based Optical Metamaterials By Doping at Atomic and Mesoscopic Lengthscales — ***Kihoon Kim****, Zachary Sherman, Angela Cleri, Jon-Paul Maria, Thomas Truskett, Delia Milliron*

2:14 Paper 327i: Mie Resonance-Enhanced Photocatalysis Using Dielectric Cuprous Oxide Nanostructures — *Ravi Teja Addanki Tirumala,* ***Sundaram Bhardwaj Ramakrishnan****, Marimuthu Andiappan*

2:27 Paper 327j: Photosensitive and Stable Hgte Quantum Dot for Mid-Wavelength Infrared Photodetector — ***Jungchul Noh****, Rich Pimpinella, Brian A. Korgel*

2:40 Paper 327k: DNA Origami for Nanoparticle Organization and Plasmonic Applications — ***Elizabeth Jergens****, Kehao Huang, Michael Poirier, Ezekiel Johnston-Halperin, Carlos E. Castro, Jessica Winter*

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(328) Synthesis and Application of Inorganic Materials II: Applications

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-122A

Gaurav Giri, Chair
Mark Snyder, Co-Chair
Meenesh Singh, Co-Chair

Sponsored by: Inorganic Materials

12:30 Paper 328a: Liquid Metal Oxide Annealing for the Simple Generation of Sensing and Electronic Materials — ***Amanda Koh****, Matthew DeBrunner, Skylar Elliott, Jordan Evans*

12:45 Paper 328b: Cation Effect to the Luminescence Performance and Temperature Sensitivity of Rare-Earth Doped Complex Metal Oxide — ***James Dorman**, Yuming Wang, Ruchi Patel*

1:00 Paper 328c: *De Novo* Protein Systems for the Controllable Biomineralization of Semiconductor Quantum Dots — ***Leah Spangler**, Michael H. Hecht*

1:15 Paper 328d: Microfluidic Studies of Colloidal Atomic Later Deposition — ***Amanda Volk**, Robert Epps, Daniel Yonemoto, Benjamin Masters, Felix N. Castellano, Milad Abolhasani*

1:30 Paper 328e: Low-Temperature Synthesis Approaches for $BaZrS_3$ — ***Jonathan Turnley**, Kiruba Vincent, Apurva Pradhan, Daniel Hayes, Madeleine Uible, Suzanne Bart, Rakesh Agrawal*

1:45 Paper 328f: Sol-Gel Synthesis of Doped (Mn, Ti)-Oxides for Asymmetric Supercapacitors — ***Khang Huynh**, Bharathkiran Maddipudi, Anuradha Shende, Rajesh Shende*

2:00 Paper 328g: Synthesis, Characterization, and Optimization of Carboxyl-Rich Oxidized Graphene Nanoplatelets Via a Simplified Hummer's Method — ***Oubayda Sras**, Grace Rushing, Rami Al-Sughayer, Hunain Alkhateb, **Sasan Nouranian**, Ahmed Al-Ostaz*

2:15 Paper 328h: Stabilized CuO for Methanol Steam Reforming to Produce Hydrogen — ***Yiwei Yu**, Jingyue Liu*

2:30 Paper 328i: Porous Phosphorus-Doped Boron Nitride Materials for Photocatalytic CO_2 Reduction — ***Ioanna Itskou**, Dave Grinter, Georg Held, Camille Petit*

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(329) Carbon Nanomaterials: Graduate Student Award Session

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, W-104B

Anju Gupta, Chair
Rebecca L. Pinals, Co-Chair

Sponsored by: Carbon Nanomaterials

12:30 Paper 329a: Photothermal Conversion Efficiency of Multi-Color Emissive Carbon Dots: Chemical and Thermal Analysis — ***Salar Balou**, Aashish Priye*

12:45 Paper 329b: Unique Thermodynamic Co-Surfactant Equilibria of Single Walled Carbon Nanotubes for Fluorescent Biosensors — ***Aniruddha Kulkarni**, Stephen Michel, Irene Chung, Claire Marc, Yang Zhao, Kirk J. Ziegler*

1:00 Paper 329c: Estimation of the Structure of Confined Water between Hybrid Materials Using Convolutional Neural Networks (CNN) — ***Abhishek Sose**, Fangxi Wang, Sanket Deshmukh*

1:15 Paper 329d: High Performance 3D Printed Faradaic Supercapacitor Using Hybrid Nanocomposites of Reduced Graphene Oxide/MnO_x-Based Electrodes — ***Mahshid Mokhtarnejad**, Erick L. Ribeiro, Dibyendu Mukherjee, Bamin Khomami*

1:30 Paper 329e: Understanding Oligonucleotide Hybridization on Single-Walled Carbon Nanotube Corona Phases for Viral Sensing Applications — ***Jianqiao Leslie Cui**, Xun Gong, Xiaojia Jin, Sooyeon Cho, Sungyun Yang, Michael Strano*

1:45 Paper 329f: Implications of Multiscale Graphene Interfaces on "Reverse" or "Inversed" Boiling — ***Seyed Alireza Rozati**, Anju Gupta*

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(330) Nanomaterials for General Electrochemical Phenomena

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, W-105C

Tae-Sik Oh, Chair
Seung Soon Jang, Co-Chair

Sponsored by: Nanomaterials for Energy Applications

12:30 Paper 330a: Synthesis and Application of the Spherical Nanoporous Carbons for Energy Conversion and Energy Harvesting — ***Chanho Pak**, Jong Gyeong Kim, Sunghoon Han, Jisue Kang, Seokjun Cha, Jong-Jin Park*

1:00 Paper 330b: Microscopic Modeling Ligand Crosslinking in Nanopatterning of Quantum Dots (QDs) — ***Niranjan Sitapure**, Tae Hyun Kwon, Jeehye Yang, Moon Sung Kang, Joseph Kwon*

1:20 Paper 330c: On the Importance of the Electric Double Layer Structure in Electrocatalysis — ***Hyungjun Kim***

1:50 Paper 330e: Tailored Mesoporous Structures of Lignin-Derived Nano-Carbons for High Performance Supercapacitors — ***Lu Yu**, David Keffer, David Harper*

2:10 Paper 330f: Heteroatom Doping in N-Coordinated Metal Site Embedded Graphene for Highly Active Oxygen Reduction Reaction — ***Ara Cho**, Jeong Woo Han*

2:40 Paper 330g: Polymer Threaded Metal Organic Frameworks with Ionic and Electrical Conductivity for Electrochemical Applications — ***Chi-Ying Vanessa Li**, Ching-Kit Ho, Liang Gao*

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(331) Nanoparticle Drug Delivery Systems

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, W-104A

Joo-Youp Lee, Co-Chair
Hannah Zierden, Co-Chair

Sponsored by:
Bionanotechnology

12:30 Paper 331a: Identifying Protein Corona Composition on Lipid Nanoparticle-Based mRNA Delivery Vehicles — ***Elizabeth Voke**, Rebecca L. Pinals, Mariah Arral, Kathryn Whitehead, Markita Landry*

12:47: Break

1:04 Paper 331c: Desolvent-Free Vaccine Platform to Enhance Effectiveness of Protein Subunit Vaccines — ***Jaeyoung Park**, Julie Champion*

1:21: Break

1:38 Paper 331e: Targeting Dysfunctional Blood-Brain Barrier Improves Nanoparticle Delivery into the Brain — *Aria W. Tarudji, Hunter A. Miller, Evan Curtis, Brandon McDonald, Badrul Alam Bony, Alex Vecchio, Punita Dhawan, **Forrest Kievit***

1:55 Paper 331f: Neonatal Pharmacokinetics and Biodistribution of Polymeric Nanoparticles — ***Nuo Xu**, Megan Wong, Elizabeth Nance*

2:12 Paper 331g: Combined Radiation-Induced Photodynamic Therapy and Immunotherapy Using Calcium Tungstate Nanoparticles, 5-Aminolevulinic Acid, and Epacadostat — ***Dhushyanth Viswanath**, Sandra Torregrosa-Allen, Haley Harper, Bennett D. Elzey, You-Yeon Won*

2:29 Paper 331h: Modified Peroxamide-Based Reactive Oxygen Species (ROS)-Responsive Doxorubicin Prodrug — ***Joo-Youp Lee**, Mina Jafari, Vishnu Sriram*

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(332) Theory, Modeling and Simulation of Nuclear Chemical Processes II

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, W-102C

Karl Hammond, Chair
Valmor de Almeida, Co-Chair

Sponsored by: Nuclear Engineering Division

12:30 Paper 332a: Helium Transport and Bubble Growth Near Grain Boundaries in Plasma-Facing Tungsten — ***Karl Hammond**, Dimitrios Maroudas, Brian D. Wirth*

12:51 Paper 332b: Hierarchical Multiscale Modeling of Surface Morphological Response of Plasma-Facing Tungsten — ***Dwaipayan Dasgupta**, Asanka Weerasinghe, Chao-Shou Chen, Sophie Blondel, Dimitrios Maroudas, Brian D. Wirth*

1:12 Paper 332c: Effect of Surface Vacancy-Adatom Pair Formation on Surface Morphological Response in Plasma-Facing Tungsten — ***Chao-Shou Chen***, *Dwaipayan Dasgupta, Asanka Weerasinghe, Karl Hammond, Brian D. Wirth, Dimitrios Maroudas*

1:33 Paper 332d: Molecular-Dynamics Analysis of the Mechanical Behavior of Plasma-Facing Tungsten — ***Asanka Weerasinghe***, *Enrique Martinez, Brian D. Wirth, Dimitrios Maroudas*

1:54 Paper 332e: Elucidating the Mechanisms of Hydrogen Blister Formation in Plasma-Facing Tungsten — ***Brandon S. Laufer***, *A. Camila Leiva, Karl Hammond*

2:15 Paper 332f: Analysis of Soret Diffusion of Helium, Hydrogen, and Intrinsic Defects in Tungsten — ***Dimitrios Maroudas***, *Dwaipayan Dasgupta, Sophie Blondel, Brian D. Wirth, Enrique Martinez*

2:36 Paper 332g: Onset of Fuzz Formation in Plasma-Facing Tungsten As a Surface Morphological Instability — ***Chao-Shou Chen***, *Dwaipayan Dasgupta, Robert Kolasinski, Brian D. Wirth, Dimitrios Maroudas*

(333) Particle Breakage and Comminution Processes

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, W-106C

Sarang Oka, Chair
Jung-Sheng Wu, Co-Chair

Sponsored by: Particle Production and Characterization

12:30 Paper 333a: Development of Multi-Dimensional Population Balance Using a Breakage Mode Classification Kernel for the Prediction of Milled Granule Quality Attributes — ***Ashley Dan***, *Rohit Ramachandran*

12:50 Paper 333b: Dry Ball Milling of a Pre-Milled Cement Clinker: Elucidating the Impact of the Ball Material Type and Size of Grinding Balls — ***Ecevit Bilgili***, *Nontawat Muanpaopong, Rajesh Dave*

1:10 Paper 333c: An Enthalpy-Balance Model for Timewise Evolution of Temperature during Wet Stirred Media Milling of Drug Suspensions — ***Gulenay Guner***, *Sherif Elashri, Mirsad Mehaj, Natasha Seetharaman, Dogacan Yilmaz, Ecevit Bilgili*

1:30 Paper 333d: Modelling Particle Aggregation and Breakage in Suspensions By Coupled CFD-DEM — *Lequan Zeng,* ***Eirini Goudeli***, *George Franks*

1:50 Paper 333e: Effect of Agitation Rate on Breakage Kinetics of Urea Crystals in Agitated Slurries — *Paras Shah,* ***Priscilla Hill***

2:10 Paper 333f: A Viscoelastic Model for Droplet Breakup in Dense Emulsions — ***Joseph Peterson***, *Vipin Michael, Ioannis Bagkeris*

2:30 Paper 333g: Polydisperse Daughter Droplet Distributions from a Binary Breakage Kernel: A Viscoelastic Model for Dense Emulsions — ***Joseph Peterson***, *Vipin Michael, Ioannis Bagkeris*

(335) Pharmaceutical Powder and Particulate Systems

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, W-106B

William Ketterhagen, Chair
Shankali Pradhan, Co-Chair

Sponsored by: Solids Flow, Handling and Processing

12:30 Paper 335a: Integration of High-Fidelity Simulation and Surrogate Modeling for Reduced Model Development in Continuous Pharmaceutical Unit Operations — ***Yingjie Chen***, ***Pooja Bhalode***, *Marianthi Ierapetritou*

12:48 Paper 335b: Breakage of Elongated Crystals in an Agitated Filter Dryer — *François S. Hallac, Frans L. Muller,* ***Andrew Bayly***

1:06 Paper 335c: DEM-Based Refill Strategy Optimization of a Twin-Screw Feeder — ***Peter Toson***, *Johannes G. Khinast*

1:24 Paper 335d: How Critical Is the Wall Cohesion for Flow of Cohesive Powders? the Cases of Tablet Press Feeder and Hopper Screw Feeder — *Ankita Sharma, Lokeshwar Mahto, Tarun De,* ***Jayanta Chakraborty***, *Anurag Tripathi, Jitendra Kumar, William Ketterhagen, Maitraye Sen*

1:42 Paper 335e: Application of Peridynamics to Predict Pharmaceutical Tablet Robustness — ***Sean Garner***, *William Ketterhagen, John C. Strong, Stewart Silling*

2:00 Paper 335f: Tribocharging Quantification to Enhance Processability — ***Filip Francqui***, *Salvatore Pillitteri, Aurelien Neveu, Geoffroy Lumay*

2:18 Paper 335g: Pharmaceutical powder compaction; an accurate finite-element representation and prediction of binary mixtures — *Danny van der Haven, Frederik H. Ørtoft, Kaisa Naelapää,* ***Ioannis Fragkopoulos***, *James A. Elliott*

2:36 Paper 335h: An Assessment of Batch Powder Bin Blending Performance Via Process Analytical Technology (PAT) and Discrete Element Method (DEM) Simulation to Predict Blend Homogeneity — ***William Ketterhagen***, *Greg Doddridge, Jeffery Larson, Leo Manley*

(336) Continuous Processing in Drug Substance: Advancements in Industry

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-123

Luke Rogers, Chair
Robert Franklin, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

12:30 Paper 336a: Continuous Flow Process Development for a Radical Chlorodifluoromethylation Reaction — ***Alexander Hesketh***, *Lu Han, Steven M. Guinness, Elaa Hilou, Ian Hotham, Robert Singer, Jordan Willie, Madison Gileau, Jason Ewers, Marcin Dembowski*

12:51 Paper 336b: Flow Chemistry As an Enabling Tool for Scale-up of API Processes — ***Detian Gao***, *Tiago Vieira, Andrew Stevens, Nick Uhlig, Andrew Martins, Lars Heumann, Andrei Chtchemelinine, Pavel Badalov*

1:12 Paper 336c: Automated Continuous Crystallization Platform — ***Kakasaheb Nandiwale***, *Kevin Girard, Robert Pritchard, Charissa Nowak, Zheng Zhao, Steven M. Guinness*

1:33 Paper 336d: Developing Around Uncertainty in the Scale up and Tech Transfer of Flow Reactions with Highly Reactive Reagents — ***Robert Franklin***, *Travis Armiger, Pratiq Patel, Douglas Otte, Jackson Hall, Reed Larson, Val Rodrigues, Holst Halsey, Lisa Jellett, Nadine Kuhl, James P. Corry, Cheol Chung*

1:54 Paper 336e: Distributed Pharmaceutical Manufacturing: The Quest for Pharmacy on Demand — ***Julian Chesterman***, *Luke Rogers, Tyler McQuade*

2:15 Paper 336f: Practical Challenges and Solutions to Continuous Grignard Chemistry — ***Sean Keenan***, *Ahmet Aloglu, Aibolat Koishybay, Stephen Born, Chuntian Hu*

2:36 Paper 336g: Enable the Implementation of Photochemical Reactions on Commercial Scale Via Using Continuous Flow Reactors — ***Hongwei Yang***

(337) Integrated Product and Process Design with Pharmaceutical Applications I

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-122C

Pablo A. Rolandi, Chair
Qinglin Su, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

12:30 Paper 337a: Optimization of Continuous Spin Freezing in Single Vial Unit By Implementing Computational Fluid Dynamics Modeling and Simulation — ***Isar Charmchi***, *Gust Nuytten, Ashish Kumar, Thomas De Beer*

12:51 Paper 337b: A System Model for a Dry-Granulated Tablet Manufactured from a Spray Dried Dispersion Intermediate: Use in Process Development and Tech Transfer — ***Salvador Garcia Munoz***, *Mehuli Kulkarni, James E. Miesle*

1:12 Paper 337c: Why Do We Dwell on Dwell Time? a Compaction Simulator Study Investigating Tableting Attributes — ***MayLin Howard***, *Gerard R. Klinzing*

1:33 Paper 337d: Uncertainty Propagation for Probabilistic Prediction in Partial Least Squares Using Bootstrap Methods — ***James Odgers***, *Chrysoula Kappatou, Ruth Misener, Salvador Garcia Munoz, Sarah Filippi*

1:54 Paper 337e: The Use of Integrated *in-Vitro-in-Silico* frameworks Toward De-Risking Low-Dose Dry Powder Inhalation Development — ***Joana Pinto***, *Snezana Radivojev, Valerie Reinisch, Eleonore Fröhlich, Amrit Paudel*

2:15 Paper 337f: Pharmaceutical HME Process Development: Understanding Non-Newtonian Fluid Flow — ***Josip Matic***, *Svetlana Marinova, Ralf Kühn, Markus Schmudde, Johannes G. Khinast*

2:36 Paper 337g: Integrated Formulation and Process Design for 3D Printing of Pharmaceuticals — ***Varun Sundarkumar***, *Zoltan Nagy, Gintaras Reklaitis*

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(338) Process Intensification – Novel Reactors (Energy Focus)

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-222A

Kishori Deshpande, Chair
Mrunmayi Kumbhalkar, Co-Chair

Sponsored by: Process Intensification & Microprocess Engineering

12:30 Paper 338a: Improved Non-Oxidative Butane Dehydrogenation Via RF Induction Heating — ***Cameron Roman***, *Foroogh Khezeli, Craig Plaisance, Kerry Dooley, James Dorman*

1:00 Paper 338b: Electrified Steam Reforming on Rh/Al_2O_3 Washcoated Open-Cell Foams: Experimental and Modeling Study — *Lei Zheng,* ***Matteo Ambrosetti***, *Francesca Zaio, Alessanda Beretta, Gianpiero Groppi, Enrico Tronconi*

1:30 Paper 338c: Piston Reactor Capabilities to Drive Endothermic Gas Reactions – a Modeling Study — ***Aya Abousrafa***, *Mamoun Al-Rawashdeh, Patrick Linke, Mary Katbeh*

2:00 Paper 338d: Microwave Enhanced CO_2 Dehydrogenation of Ethane over Supported Transition Metal Carbides — ***Brandon Robinson***, *Ashley Caiola, Sean Brown, Jianli Hu*

2:30 Paper 338e: Analysis of an Integrated Photoelectrochemical Redox Flow Device for Brackish Water Desalination Using a Dye-Sensitized Photoanode — ***Sitaraman Krishnan***, *Gowri Mohandass, Taeyoung Kim*

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(339) Adsorbent Materials

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-131C

Roger D. Whitley, Chair
Masoud Jahandar Lashaki, Co-Chair

Sponsored by: Adsorption and Ion Exchange

12:30 Paper 339a: Synthesis and Characterization of Isomorphically Substituted Alpo-5 Zeolites for Oxygen Adsorption — ***Natalia Ali***, *Steven Wilson, Ellen B. Stechel, Ivan Ermanoski, Andrea Ambrosini, Christopher L. Muhich, Shuguang Deng*

12:48 Paper 339b: Developing Hierarchical Silica-Salt Composites Via Wet Impregnation for Atmospheric Water Harvesting from Arid Air — ***Jamie Salinger***, *Carmen Chen, Molly Essig, Krista Walton*

1:06 Paper 339d: Atomic Layer Deposited Dual-Function Materials for Combined Adsorption and Oxidation of VOCs — *Busuyi Adebayo, Ali Rownaghi,* ***Fateme Rezaei***

1:24 Paper 339e: Modification of Zeolites with Organic Phosphonic Acids for Adsorptive Separation of Gases — ***Xinpei Zhou***, *John L. Falconer, J. Will Medlin*

1:42 Paper 339f: Effect of SO_2 on CO_2 Capture Performance of Self-Supported Branched Poly(ethyleneimine) Scaffolds — ***Pavithra Narayanan***, *Chun-Jae Yoo, Ryan P. Lively, Christopher W. Jones*

2:00 Paper 339g: CO and CO2 Adsorption by a New ZSM-5@MOF-199 Composite Adsorbent — ***Farshad Feyzbar-khalkhali-Nejad***, *Ehsan Hassani, Katie D. Leonard, Samuel Sessions, Morteza Taghavi Kouzehkanan, Tae-Sik Oh*

2:18: Break

2:36 Paper 339i: Alkyl Amine Incorporation in Functional and Processible Porous Organic Polymers for CO_2 Capture Applications — ***Ali Sekizkardes***, *Victor A. Kusuma, Jeffrey Culp, Patrick Muldoon, James S. Hoffman, David Hopkinson*

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(340) Advances in Bioseparations

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-130

Christoph Brandenbusch, Chair
Tim Zeiner, Co-Chair

Sponsored by: Bio Separations

12:30 Paper 340a: Adaptive Laboratory Evolution and Rational Engineering Enables Osmolysis-Based Recovery of Biomacromolecules from *Cupriavidus Necator* — ***Jeremy Adams***, *Douglas S. Clark*

12:48 Paper 340b: Isolation Strategies Based on Membrane Processes for Extracellular Vesicles from *Citrus Limon* — *Sara Giancaterino, Mariaelena Schiavone,* ***Cristiana Boi***

1:06 Paper 340c: Confocal and Multiphoton Imaging of IgG Gel Layer Formation during Tangential Flow Filtration — ***Fernanda Cunha***, *Francesco Rossi, Eduardo Ximenes, Norvin Bruns, Ken K. Qian, McKensie Mason, Brian D. Bowes, Zhao Yu, Dennis T. Yang, Vincent Corvari, Arezoo Ardekani, Gintaras Reklaitis, Michael Ladisch*

1:24 Paper 340d: Predicting Biomolecule Partitioning in Aqueous Two-Phase Systems through Thermodynamic Modeling — ***Maximilian Wessner***, *Christoph Brandenbusch*

1:42 Paper 340e: Enzyme Purification and Sustained Enzyme Activity By Fusion with Phase-Separating Intrinsically Disordered Protein — ***Xinyi Li***, *Augene Park, Grant S. Murphy, Karla Camacho Soto, Benjamin S. Schuster*

2:00 Paper 340g: ChromaWeb™ platform, a linearly-scalable, high-resolution membrane chromatography cassette for purification of viral vectors. — ***Gastón de los Reyes***, *Erik Blomquist, Danielle Marquis*

2:18 Paper 340h: How to Drive a Bio Macromolecule DNA Faster through Nano Pores — ***Aniruddha Deb***, *Dr. Partho S.G. Pattader*

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(341) Crystallization of Pharmaceutical and Biological Molecules

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-131A

Fredrik Nordstrom, Chair
Richard D. Braatz, Co-Chair
Marina Tsianou, Co-Chair

Sponsored by: Crystallization and Evaporation

12:30: Introductory Remarks

12:33 Paper 341a: Streamlining Crystallization Process for a Low Solubility and Highly Solvating API System to Achieve Robust Scale-up Performance — *Shujauddin Changi,* ***Andrew McTiernan***, *Stefanie Roeper, Mei-Hsiu Lai, Christian Zeigler, Hanyu Zhu, Adam Looker, David Willcox*

1:02 Paper 341c: Interfacial Structure and Dynamics of Aqueous-Organic Solvent Illuminates the β-Hematin Crystallization Mechanism — ***Lakshmanji Verma***, *Peter Vekilov, Jeremy Palmer*

1:31 Paper 341d: An Approach to Achieve Clarifying Filtration for the Reactive Crystallization of Poorly Soluble Organic Salts — ***Lotfi Derdour***, *Weiling Cai*

2:00 Paper 341e: Enabling Crystallization for a Challenging Active Pharmaceutical Ingredient through Use of a Wet-Milling Crystallization Process at Elevated Temperature — ***Christopher Marton***, ***Zhiwei Yin***, *Tamar Rosenbaum, Deniz Erdemir, Junhe Ma*

2:29: Concluding Remarks

(342) Honorary Session for Prof. Suzana Nunes III

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-131B

Dibakar Bhattacharyya, Chair
Isabel Escobar, Co-Chair
Lakshmeesha Upadhyaya, Co-Chair
Cristiana Boi, Co-Chair

Sponsored by: Membrane-Based Separations

12:30 Paper 342a: Design and Synthesis of Polymer Membranes Based on Theoretical Principles — *Mirco Sorci, Surya Karla, Chenyu Guan, Corey Woodcock, Dustin J. Andersen, Ali Reza Behzad, Suzana Nunes, Joseph Hersey, Lauren Tice, Sal Giglia, Joel Plawsky,* ***Georges Belfort***

12:50 Paper 342b: Novel Strategy to Control the Pore Structure and Surface Chemistry of Cellulose-Based Carbon Molecular Sieve Membranes — *Tiago Araújo, Francisco Barbosa, Gabriel Bernardo,* ***Adélio Mendes***

1:10 Paper 342c: Cellulose-Cellulose Composite Membranes for Ultrafiltration — ***Mathias Ulbricht***, *Duc Hoa Tran*

1:30 Paper 342d: Self-Assembly of Zwitterionic and Charged Random Copolymers for Membranes with Exceptional Performance — ***Ayse Asatekin***

1:50 Paper 342e: 3D Printed Nanofiltration Composite Membranes with Reduced Concentration Polarisation — ***Davide Mattia***

2:10 Paper 342f: Challenges to Tackle with Membrane Science for a More Sustainable Future — ***Suzana Nunes***

(343) Membrane Modeling and Simulation

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-132A

Xianghong Qian, Chair
Nitish Mittal, Co-Chair

Sponsored by: Membrane-Based Separations

12:30 Paper 343a: Effect of Molecular Dynamics Water Models on Flux and Diffusivity in Membranes — *Suwei Liu, Sinan Keten,* ***Richard Lueptow***

12:51 Paper 343b: Optimization Based Modeling and Analysis of Osmotically Assisted Reverse Osmosis for Application in Shale Oil and Gas Produced Water Treatment — ***Elmira Mohammadi Shamlou***, *Radisav Vidic, Vikas Khanna*

1:12 Paper 343c: Design Driven Trends in Transport and Stability of Biomimetic Membranes with Highly Selective Water Channels — ***Ritwick Kali***, *Erha Andini, Scott T. Milner*

1:33 Paper 343d: Mitigated Carrier Saturation of Facilitated Transport Membranes for Decarbonizing Dilute CO_2 Sources — ***Yang Han***, *W.S. Winston Ho*

1:54 Paper 343e: A Model for the Separation of Complex Liquid Mixtures with Glassy Polymer Membranes: A Thermodynamic Perspective — ***Bennett Marshall***, *Joshua Allen, Ryan P. Lively*

2:15 Paper 343f: Moisture Driven Pump to Concentrate CO2 from Air — ***Jennifer Wade***

2:36 Paper 343g: A Spatiotemporal Model for Dynamic RO Simulations — ***Mingheng Li***

(344) Biofuels Production: Design, Simulation, and Economic Analysis

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-226B

Ana I. Torres, Chair
Ramalingam Subramaniam, Co-Chair

Sponsored by: Sustainable Biorefineries

12:30 Paper 344a: Sustainable Biofuels for Low-Carbon Maritime Transportation — ***Eric Tan***, *Abhijit Dutta, Kristiina Iisa, Calvin Mukarakate*

12:45 Paper 344b: Bipolar Hydrogen Production from Biorenewable Aldehydes and Water in Membrane-Less Electrolyzers — *Hengzhou Liu, Naveen Agrawal, Arna Ganguly, Yifu Chen, Jungkuk Lee,* ***Wenzhen Li***, *Mark Mba Wright, Michael J. Janik*

1:00 Paper 344c: Economic and Environmental Potentials of Biofuel Production Process Using Biphasic Reactor - Cyclopentyl Methyl Ether As Organic Solvent for Xylose Upgrading. — ***Kyeongsu Kim***, *Jinjoo An, Young-Woong Suh, Jeong-Myeong Ha, Ung Lee*

1:15 Paper 344d: Uncertainties in Economic and Environmental Analyses of Wet Waste Hydrothermal Liquefaction Process for Fuel Production — ***Yuan Jiang***, *Lesley J. Snowden-Swan, Chirag Mevawala, Shuyun Li, Andrew J. Schmidt, Justin M. Billing, Michael R. Thorson*

1:30 Paper 344e: Optimal Design of an Integrated Cyanobacteria-Based Biorefinery for Biofuels, PHAs and Bioproducts Production and Simultaneous Synthesis of Its Hen — *Matias Ramos, Romina Lasry Testa, Fernando Ramos, Vanina Estrada,* ***Maria Soledad Diaz***

(345) Concentrated Solar Power Generation and Chemical Processing II

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-226C

Christopher Muhich, Chair
Alexandre Yokochi, Co-Chair
Wojciech Lipinski, Co-Chair
Nick AuYeung, Co-Chair
Ashley Pennington, Co-Chair

Sponsored by: Sustainable Energy

12:30 Paper 345a: Sustainable Ammonia Production with an Advanced Solar Thermochemical Cycle: Techno-Economic Analysis — ***Alberto de la Calle***, *H. Evan Bush, Ivan Ermanoski, Andrea Ambrosini, Ellen B. Stechel*

12:48 Paper 345b: Overcoming Challenges in Off-Stoichiometric Thermodynamics Modeling through Complementary Use of Experimental and First Principles Data: A Case Study of $Ba_{1-x}Sr_xFeO_{3-\delta}$ — ***Steven Wilson***, *Ellen B. Stechel, Christopher L. Muhich*

1:06 Paper 345c: Mathematical Modelling of an Enhanced Volumetric Solar Receiver Based on Partially Reflective Surfaces with a Discussion on the Volumetric Effect Criteria — *Fathya Salih,* ***Konstantinos E. Kakosimos***, *Athanasios G. Konstandopoulos*

1:24 Paper 345d: Design of a Combined Moving-Fluidized Bed Oxidation Reactor for High Temperature Solid-State Thermochemical Energy Storage — ***Juvenal Ortiz-Ulloa***, *Fuqiong Lei, Lucas Freiberg, Nesrin Ozalp, Like Li, Kelvin Randhir, Joerg Petrasch, James F. Klausner, Nick AuYeung*

1:42 Paper 345e: Geometry design and thermodynamic analysis of an epitrochoidal rotary reactorfor solar hydrogen production via ceria redox cycle — ***Bo Wang***, *Xian Li, Yanjun Dai, Chi-Hwa Wang*

2:00 Paper 345f: Process Optimization of Calcium-Looping for Concentrating Solar Power Plants — ***Diogo Rodrigues***, *Carla Pinheiro, L. Filipe Mendes*

2:18: Break

2:36 Paper 345h: Enhanced Radiative Heat Transfer of Concentrated Solar Energy in Hierarchically Ordered Porous Structures — ***Sebastian Sas Brunser***, *Hugo Braun, Roxanne Vandenberghe, Fabio Luca Bargardi, Rafael Libanori, André R. Studart, Aldo Steinfeld*

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(346) The Food-Energy-Water Nexus

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-226A

Yuan Yao, Chair
Vikas Khanna, Co-Chair
M M Faruque Hasan, Co-Chair

Sponsored by: Sustainability Science and Engineering

12:30 Paper 346a: Socio-Ecological Network Structures from Process Graphs in the Context of the Food-Energy-Water Nexus — *Angelyn Lao, Kathleen Aviso,* ***Heriberto Cabezas****, Raymond Tan*

12:45 Paper 346b: Impact of the Food-Energy-Water Nexus on Meeting the Constraints of Planetary Boundaries and Social Justice — ***Yazeed Aleissa****, Bhavik Bakshi*

1:00 Paper 346c: Dynamics of Sustainable Agriculture & Food Supply Chains — ***John Starr***

1:15 Paper 346d: Evaluation of Global Techno-Socio-Economic Policies for the FEW Nexus with an Optimal Control Based Approach. — ***Apoorva Nisal****, Urmila Diwekar, Neeraj Hanumante, Yogendra Shastri, Heriberto Cabezas, Vicente Rico-Ramirez, Pablo T. Rodríguez-González*

1:30 Paper 346e: Sustainable Agriculture Sprays: Cellulose Ester Aqueous Dispersions As Rainfast Biodegradable Foliar Formulations for Targeted Agrochemical Delivery — ***Mariam Sohail****, Tahira Pirzada, Saad A. Khan, Charles H. Opperman*

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(347) Topical Plenary: Topical Conference in Molecular and Materials Data Science (Invited Talks)

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-124AB

Johannes Hachmann, Chair

Sponsored by: Applications of Data Science to Molecules and Materials

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(348) Pandemic Response and Public Health

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-126C

Christopher Burcham, Chair
Leonard Pease, Co-Chair

Sponsored by: Chemical Engineers in Medicine

12:30 Paper 348a: Indoor Transport of Aerosolized Respiratory Droplets in Multiroom Buildings — *Alex Vlachokostas, Timothy Salsbury, Carolyn A. Burns,* ***Leonard Pease***

12:54 Paper 348b: Multi-Strain Integrated Modelling for COVID-19 — ***Dimosthenis Sarigiannis****, Achilleas Karakoltzidis, Spyros Karakitsios*

1:15 Paper 348c: Portable and Label-Free Quantitative Loop-Mediated Isothermal Amplification (LF-qLamp) for Reliable COVID-19 Diagnostics in Three Minutes of Reaction Time — ***Sergio Bravo-González****, Grissel Trujillo de Santiago, Mario Moisés Álvarez*

1:36 Paper 348d: Affordable Rapid PCR-Based Biodetection at the Point of Care Via Rayleigh-Bénard Convection — ***MinGin Kim****, Victor Ugaz*

1:57: Break

2:18 Paper 348f: Rapid Bioproduction of Protein Biologics Using Plants in Response to Sars-Cov-2 — ***Katherine Haddad****, Seongwon Jung, Imran Khan, Nancy E. Lane, Somen Nandi, Karen A. McDonald*

2:39 Paper 348g: Strategic Planning of Joint COVID-19 Booster and Influenza Vaccination Campaign: The UK COVID-19 Pandemic Study — ***Dauda Ibrahim****, Zoltán Kis, Maria Papathanasiou, Cleo Kontoravdi, Benoit Chachuat, Nilay Shah*

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(349) Interfacial Systems for Energy Application: Experimental Validation

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-227A

Yuzhang Li, Chair
Joaquin Resasco, Co-Chair

Sponsored by: Material Interfaces as Energy Solutions

12:30 Paper 349b: Advancing Quantitative Understanding of Functionality in the Lithium SEI in Liquid Electrolytes — ***Betar Gallant***

12:55 Paper 349c: On-Line Flow Cell Trace Elemental Analysis Elucidates Degradation Mechanisms in Transition Metal Oxygen Electroreduction Catalysts — ***Gaurav A. Kamat****, Sanzeeda Shuchi, Melissa Kreider, Jose A. Zamora Zeledon, Michaela Burke Stevens, Thomas Jaramillo*

1:20 Paper 349d: Exploring How Interfacial Ion Assembly Accelerates Electrochemical CO_2 Reduction — ***Matthew Gebbie****, Beichen Liu, Wenxiao Guo*

1:45 Paper 349e: Interface Lithiophobicity Regulation for Lithium Metal Solid-State Batteries — ***Xinzi He****, Xiao Ji, Chunsheng Wang*

2:10 Paper 349f: Dynamic Photo-Electrochemical Interface for Solar Fuels — ***Weilai Yu****, Nathan S. Lewis*

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(350) Modeling, Optimization, and Control in Next-Gen Manufacturing I

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-221A

Amir Barati Farimani, Chair
Q. Peter He, Co-Chair

Sponsored by: Next-Gen Manufacturing

12:30 Paper 350a: Control-Theoretic Considerations for Manufacturing in Space — ***Kip Nieman****, Katie Tyrrell, Helen Durand*

12:55 Paper 350b: Some of the Variables, Some of the Times, with Some Things Known: Identification with Partial Information — ***Saurabh Malani****, Thomas Bertalan, Tianqi Cui, Michael Betenbaugh, Jose Avalos, Ioannis G. Kevrekidis*

1:20 Paper 350c: Intersecting Quantum Computing and Control with Materials — ***Jihan Abou Halloun****, Keshav Kasturi Rangan, Henrique Oyama, Helen Durand*

1:45 Paper 350d: Generalizing Physics-Informed Neural Networks to Unseen Boundary and Initial Conditions — ***Zachary Kilwein****, Fani Boukouvala*

2:10 Paper 350e: Use of Computational Fluid Dynamics (CFD) Modelling to Optimize Continuous Mixer Design — ***Chang Kai Wu****, Marc Thibaut*

2:35 Paper 350f: Verification of Neural-Network-Based Explicit Control Systems Using Mixed-Integer Programming — ***Calvin Tsay****, Jan Kronqvist, Alexander Thebelt, Ruth Misener*

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(351) Polymers in Additive Manufacturing

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-221B

Emily Davidson, Chair
Jinhye Bae, Co-Chair

Sponsored by: 3D Printing

12:30 Paper 351a: Fabrication of Hierarchical Sorbents By a Combined 3D-Printing and in-Situ Phase Separation Process from Carbon Nanotube-Enriched Polymer Solutions — ***Jialing Xu****, Cheryl Slykas, Adam Braegelman, Kevin Gabriel Alvarez, Thomas Kasl, Matthew Webber, Vivek Sharma, Bryan Boudouris, William Phillip*

12:50 Paper 351b: 3D Printing of a Recycled Terephthalic Acid-Based Copolyester Containing Tetramethylcyclobutanediol — ***Samarthya Bhagia**, Surbhi Kore, Sanjita Wasti, Jaroslav Durkovic, Jan Kovac, Xianhui Zhao, Uday Vaidya, Soydan Ozcan, Arthur Ragauskas*

1:10 Paper 351c: Single-Digit Micron CLIP 3D Printing, Modeling and Applications — ***Kaiwen Hsiao**, Gabriel Lipkowitz, Eric Shaqfeh, Joseph M DeSimone*

1:30 Paper 351d: Additive Manufacturing Using Olefin Metathesis — ***Samuel Leguizamon**, Adam Cook, Leah Appelhans, Jeffrey Foster*

1:50 Paper 351e: Pressure-Based Process Monitoring of Direct-Ink Write Additive Manufacturing — ***Jessica Kopatz**, Derek Reinholtz, Jonathan Leonard, Alexander Tappan, Adam Cook, Anne M. Grillet*

2:10 Paper 351f: Versatile Additive Manufacturing of Microscale Metals and Alloys Via Hydrogel Infusion — *Max Saccone, Daryl Yee, Rebecca Gallivan, **Kai Narita**, Julia R. Greer*

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(352) Topical Plenary: Environmental Analytical Technology: Sensor Applications in Sustainability (Invited Talks)

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-229AB

Ariel Furst, Chair
Stephanie McCalla, Co-Chair

Sponsored by: Sensors for Sustainability

12:30 Paper 352a: Introduction to Plenary Session — ***Ariel Furst***

12:40 Paper 352b: Skin-Inspired Sensors for Human Body, Brain and Gut — ***Zhenan Bao***

1:15 Paper 352c: Susan TBD — ***Susan Daniel***

1:50 Paper 352d: Polymer-Based Sensors to Monitor Indoor Air Quality and Ocular Response — ***Bryan Boudouris***

2:25 Paper 352e: Functional Biosensors for Human and Environmental Health — ***Ariel Furst***

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(353) Sustainable Pathways to Clean Hydrogen and Synthetic Fuels II

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, W-103B

William Gibbons, Chair
Eric Miller, Co-Chair

Sponsored by: Sustainable Pathways Toward Hydrogen and Synthetic Fuels

12:30 Paper 353a: Closing the Carbon Cycle in the Shipping Industry — ***Margarita Charalambous**, Valentina Negri, Valentin Kamm, Gonzalo Guillén-Gosálbez*

12:55 Paper 353b: Economic and Environmental Assessment of Fischer-Tropsch Electro-Diesel from Captured CO_2 — ***Juan D. Medrano-García**, Margarita Charalambous, Gonzalo Guillén-Gosálbez*

1:20 Paper 353c: Modeling of an Integrated Fischer-Tropsch Process with Energy Supplied By a Nuclear Power Plant — *Guiyan Zang, Pingping Sun, **Hernan E. Delgado**, Vincenzo Cappello, Clarence Ng, Amgad Elgowainy*

1:45 Paper 353d: A Technoeconomic Assessment of Liquid Green Hydrogen Carrier Supply Chains for Delivering Sustainable Fuel — ***Bradie S. Crandall**, Todd Brix, Robert Weber, Feng Jiao*

2:10 Paper 353e: Thermal Hydrolysis of Solid-State Sodium Borohydride — *Geo-Jong Kim, **Hyun Tae Hwang***

2:35 Paper 353f: Performance of Cyclic Hydrogenation and Dehydrogenation of Benzyltoluene As Liquid Organic Hydrogen Carrier (LOHC) — ***Timo Rüde**, Patrick Preuster, Moritz Wolf, Peter Wasserscheid*

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(354) Transport In Advanced Fuel Cell Technologies

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-227B

Gang Wu, Chair
Jacob Spendelow, Co-Chair

Sponsored by: Transport and Energy Processes

12:30 Paper 354a: Novel Electrode Structures for Enhanced Transport — ***Jacob Spendelow***

1:00 Paper 354b: Improving Performance and Durability of Polymer Electrolyte Fuel Cell Cathodes with High Oxygen Permeability Ionomer — ***Shawn Litster***

1:30 Paper 354c: Recent Advances in Electrospun Fiber Mat Electrode MEAs for Hydrogen/Air Fuel Cells — *Xiaozong Fan, Xiaomin Xu, Narae Kang, R. Wycisk, **Peter Pintauro***

1:50 Paper 354d: The Impact of Inorganic Electrocatalyst Surface Ligands on Humidification Requirements in Operating Proton Exchange Membrane Fuel Cells — *Ian Moorhead, John Williams, **Anastasios Angelopoulos***

2:10 Paper 354e: Impact of Droplet/Bubble Growth Dynamics on Electrode Limiting Current — ***John Petrovick**, Arthur Dizon, Clayton Radke, Adam Weber*

2:30 Paper 354f: A DFT+U Study of the Electrochemical Oxidation of H_2 and CO on $SrLaFeO_4$ — ***Nicholas Szaro**, Andreas Heyden*

2:45 Paper 354g: Durable and Highly Active PGM-Free Cathode Catalysts in Competition with Platinum for Pemfcs — ***Gang Wu***

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(356) Meet the Industry Candidates Poster Session: Particle Technology Forum

Tuesday, Nov 15, 1:00 PM
Phoenix Convention Center, North Hall E

Ben Freireich, Chair
James Gilchrist, Co-Chair
SB Reddy Karri, Co-Chair

Sponsored by: Meet the Candidates Poster Sessions

Poster 356a: Targeted Groundwater Remediation Using Engineered Colloids — ***Joanna Schneider**, Rodney Priestley, Sujit Datta*

Poster 356b: Reversible Association of Sequence-Defined Oligocarbamates — ***R. Kenton Weigel**, Christopher Alabi*

Poster 356c: Molecular Modeling and Machine Learning-Based Design and Discovery of Nanoporous Materials for Energy and Environmental Applications — ***Krishnendu Mukherjee***

Poster 356d: Enhancing the Capture Efficiency of Antibody-Antigen Reactions in Sessile Droplets and the Study of Resultant Deposition Patterns — ***Vidisha Singh Rathaur**, Nachiket Ashish Gokhale, Siddhartha Panda*

Poster 356e: Modeling the Rheology of Aggregating Colloidal Suspensions: Insights from Population Balances and Non-Equilibrium Thermodynamics — ***Soham Jariwala***

Poster 356f: Thermodynamic and Kinetic Factors Influential in the Redispersion of Pt-Group Metal Nanoparticles to Ion-Exchanged Cations in Zeolites — ***Keka Mandal**, Christopher Paolucci*

Poster 356g: Structure-Property-Performance of Electrically Conductive Nanocomposites — ***Farivash Gholamirad***

Poster 356h: Controlling Polymorphism and Orientation of Nu-901/Nu-1000 Metal–Organic Framework Thin Films — ***Prince Verma**, Luke Huelsenbeck, Asa Nichols, Timur Islamoglu, Helge Heinrich, Charles Machan, Gaurav Giri*

Poster 356i: Adhesion of Soft Materials to Wet, Compliant or Rough Substrates — ***Preetika Karnal***

Poster 356j: Sensitivity of Ethylene Oligomerization Rates and Selectivities to the Nature of Metal Ion on Siliceous Supports By First Principles and Microkinetic Interrogation — ***Neha Mehra**, Galiya Magazova, Nicole LiBretto, Jeffrey T. Miller, Guanghui Zhang, Jason Hicks, William Schneider*

Poster 356k: Bio-Derived Dioxolanes As Renewable Diesel Fuel — ***Xiaokun Yang***

(357) Meet the Industry Candidates Poster Session: Pharmaceutical Discovery, Development and Manufacturing Forum

Tuesday, Nov 15, 1:00 PM
Phoenix Convention Center, North Hall E

Andreas Bommarius, Chair

Sponsored by: Meet the Candidates Poster Sessions

Poster 357a: Solution Deposited Synthesis of Chalcogenide Perovskites at Temperatures below 600°C — ***Apurva Pradhan***, *Shubhanshu Agarwal, Madeleine Uible, Suzanne Bart, Rakesh Agrawal*

Poster 357b: Free Energy Calculation with Non-Uniform Windows for Improved Computational Efficiency: A Proof of Concept — ***Naveen Vasudevan***, *Dongyang Li, Li Xi*

Poster 357d: Effects of Intratumoral Heterogeneity on Metastasis of Triple-Negative Breast Cancer Cells — ***Molly Brennan***, *Susan E. Leggett, Sophia Martinez, Celeste M. Nelson*

Poster 357e: Design of Functionalized Membranes for Advanced Filtration Processes — ***Alexandra Khlyustova***

Poster 357f: Development of Cationic PAMAM Dendrimers As an Avascular Tissue Drug Delivery Platform — ***Brandon Johnston***, *Simone Douglas-Green, Joon Ho Park, Alan Grodzinsky, Paula T. Hammond*

Poster 357g: Development and Evaluation of Data-Driven Control Strategies for Drying End-Point Determination in a Semi-Continuous Fluid Bed Granulation Process — ***Shashwat Gupta***, *Joshua Hanson, Adam S. Butterbaugh, Maitraye Sen*

Poster 357h: Modeling Functional Nanoporous and Soft Colloidal Materials Using Molecular Simulations and Machine Learning — ***Raghuram Thyagarajan***

Poster 357i: Fourier Transform Infrared Spectroscopy (FT-IR) of Lyophilized RNA — ***Aswathy Balakrishnan***, *Caio H.N. Barros, Jerry Sellors, Robert Packer, Steven Ferguson, Elizabeth M. Topp*

Poster 357j: High Pressure Chemistry in Manufacturing Fuel and Materials — ***Wenjia Wang***

Poster 357k: Improving Wound Infection Treatment through Sprayable, Antimicrobial Hydrogels — ***Riannon Smith***

Poster 357l: Development of Calcium Tungstate Nanoparticle Formulations for Concomitant Multimodal Treatment of Cancers — ***Dhushyanth Viswanath***

Poster 357m: Bioprocess Development of Engineered Anti-CD276/CD47 Antibody-Drug Conjugates for Cancer Treatment — ***Yingnan Si***, *Kai Chen, Yuanxin Xu, Seulhee Kim, Xiaoguang Liu*

Poster 357n: Engineering *Saccharomyces Cerevisiae* to Mimic B Cell Antibody Diversification for the Rapid Enhancement and Selection of Antibody Therapeutics. — ***Andrew Cazier***, *John Blazeck*

Poster 357o: Demonstrating the Impact of Shear and Surface Roughness on Thrombosis in Ventricular Assist Devices — ***Anjana Jayaraman***, *Junhyuk Kang, James Antaki, Brian Kirby*

Poster 357p: Computational Investigation of the Kinetics and Thermodynamics of Crystal Nucleation — ***Pelin Su Bulutoglu***

Poster 357q: Elucidating Structure-Property Relationships at Metal-Metal Oxide Interfaces for Heterogeneous Catalysis. — ***Kaustubh Sawant***

Poster 357r: Screening Solvents for Desired Polymorph Selection: A Solution Thermodynamics Study — ***Rupanjali Prasad***, *Stefani Kocevska, Dimitri Skliar, Martha Grover, Ronald Rousseau*

Poster 357s: Microfluidic Devices for Pharmaceutical Development: Lipid-Based Drug Production & Target-Directed Ligand Screening — ***Wan-Zhen Lin***, *Noah Malmstadt*

Poster 357t: Bioreactors : Mixing and Hydrodynamic Evaluation Using Computational Fluid Dynamics — ***Deepak Jain***

Poster 357u: A Comparative Study of Protein-a Membranes for the Rapid Purification of Monoclonal Antibodies — ***Joshua Osuofa***, *Scott Husson*

Poster 357v: Carbon Nanotube-Protein Conjugate for Photothermal Therapy Combined with Checkpoint Inhibition for the Immunomodulatory Treatment of Metastatic Breast Cancer — ***Gabriela Faria***, *Clément G. Karch, Adam Aissanou, Alexis Woodward, Roger Harrison*

Poster 357w: Metabolic Modeling and Systems Biology Characterization in the Green Alga *Chromochloris Zofingiensis* — ***Michelle Meagher***, *Nanette Boyle*

Poster 357x: Computational Design of HIV-1 Entry Inhibitors — ***Mohammadjavad Mohammadi***

Poster 357y: Microfluidic Approach to Dampen Stochasticity in Crystalline Drug Release and Cellular Dynamics of Senescent Mesenchymal Stem Cells — ***Ryan Miller***, *Hyunjoon Kong*

Poster 357z: *Self-Assembled Recombinant Protein Nanomaterials for Treatment of Sars-Cov-2* — ***Rajarshi Chattaraj***, *Daeyeon Lee, Daniel A. Hammer*

Poster 357aa: Structural Characterization of an Effector-Biasing IL-2 Immunocytokine — ***Joseph Gould***, *Elissa Leonard, Jamie Spangler*

Poster 357ab: Nanomaterial Synthesis Using Jet Mixing Reactor — ***Faiz Khan***, *Jessica Winter*

Poster 357ac: Active Learning Guided Discovery of Redox Active Molecules for Non-Aqueous Redox Flow Batteries — ***Akash Jain***, *Rajeev Assary*

Poster 357ae: Bio-Instructive Scaffolds for Rapid In Vivo Manufacture of CAR T Cells — ***Pritha Agarwalla***

Poster 357af: Transport and Stability of Biomimetic Membranes with Highly Selective Water Channels — ***Ritwick Kali***, *Erha Andini, Scott T. Milner*

Poster 357ag: Computational Inverse Design of Multifunctional Surfaces to Control Water and Solute Behavior — ***Sally Jiao***, *Audra DeStefano, Daniela Rivera Mirabal, Rachel Segalman, Songi Han, M. Scott Shell*

Poster 357ah: Integration of Nanoparticles and DNA Nanotechnology with Applications in Energy and Imaging — ***Elizabeth Jergens***, *Jessica Winter*

Poster 357ai: Development of Tandem Systems for Carbon Dioxide and Carbon Monoxide Electroreduction — ***Sean Overa***, *Feng Jiao*

Poster 357aj: Choreographing Zeolite Crystallization: It Is All Elementary — ***Adam J. Mallette***, *Sungil Hong, Giannis Mpourmpakis, Jeffrey Rimer*

Poster 357ak: Bio-Compatible Polymer-Conjugated Extracellular Mega-Hemoglobin for Diverse Oxygen Therapeutic Applications — ***Chintan Savla***

Poster 357al: Effect of Zwitterionic Molecules on Ionic Solvation and Transport in Electrolytes — ***Manh Tien Nguyen***, *Qing Shao*

Poster 357am: Hemoglobin Encapsulated Metal Organic Framework Nanoparticles As an Oxygen Therapeutic with Tunable Size Distribution — ***Xiangming Gu***, *Andre Palmer*

Poster 357an: Design Parameters for Water-Responsive Protein Block Copolymers — ***Jacob Kronenberg***, *Yeojin Jung, Maria Kulapurathazhe, Jason Chen, Xi Chen, Raymond S. Tu, Jin Kim Montclare*

Poster 357ao: Soybean Hull As an Alternative Source for Manufacturing Pharmaceutical Grade Microcrystalline Cellulose — ***Navid Etebari Alamdari***, *Burak Aksoy, Jayachandra B. Ramapuram, Zhihua Jiang*

Poster 357ap: Designing Life-Cycle Networks, Chemical Reaction Pathways & Innovation Roadmaps for a Sustainable Circular Economy — ***Vyom Thakker***

Poster 357aq: A Laboratory Scale Continuous Reactor for Electrochemical Phosphate Recovery from Wastewater — ***Ruhi Sultana***, *Lauren F. Greenlee*

Poster 357ar: Liposome and Polyelectrolyte Layers Derived Single Shot Vaccine Platform for Controlled Release of Inactivated Chikungunya Virus — ***Rashi Porwal***, *Anuj Sharma, Srivatsan Kidambi*

Poster 357as: Controlling the Properties of the Light Responsive Transmembrane Protein Proteorhodopsin in Mesostructured Silica-Surfactant Hybrid Materials — ***Maxwell Berkow***, *Songi Han, Bradley F. Chmelka*

Poster 357at: Application of First-Principles Calculations and Experiments in Heterogeneous Catalysis: Emission Control and Methane Valorization — ***Surya Pratap Solanki***, *Lars Grabow*

Poster 357au: Towards a More Sustainable Chemical Process Industry: Rational Design of Catalysts with Process Intensified Technologies for Applications in Heterogeneous Catalysis — ***Sanjana Karpe***, *Goetz Veser*

Poster 357av: Development of an improved α-amino ester hydrolase for the continuous reactive crystallization of β-lactam antibiotics — ***Colton Lagerman***, *Martha Grover, Ronald Rousseau, Andreas Bommarius*

Poster 357aw: Understanding interfacial composition and structure of lipid-based surfactant monolayers for treatment of pulmonary diseases — ***Julia Fisher***, *Todd Squires*

Poster 357ax: Microscale Steering of Colloids via Chemical Gradients — ***Parth Shah***

Poster 2jz: Elucidating the role of network topology dynamics on the coil-stretch transitionhysteresis in extensional flow of entangled polymer melts — ***Mahdi Boudaghi***

Poster 357ay: Continuous Enzymatic Reactive Crystallization of Beta-lactam Antibiotics — ***Patrick Harris***

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(358) Andrew Chase Award I (Invited Talks)

Tuesday, Nov 15, 2:00 PM
Phoenix Convention Center, N-228A

Xuejun Pan, Chair

Sponsored by: Forest and Plant Bioproducts Division

2:00 Paper 358a: Maleic Acid Hydrotropic Fractionation: Effective Deconstruction of Lignocellulose for Multi-Products Biorefinery — ***Junyong Zhu***

2:30 Paper 358b: Advances in Biomass Processing Solvents in Biorefinery Concept — ***Chang Geun Yoo***

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(359) Tools and Techniques for Sustainable/Green Product Design

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-221C

Mrunmayi Kumbhalkar, Chair
Shaibal Roy, Co-Chair
Sitaraman Krishnan, Co-Chair

Sponsored by: Product Design

3:30 Paper 359a: Dynamic Simulation and Optimization of Hydrogen Fueling Operated By Real-Time-Responding without Look-up Tables: 3-Bank Cascade Fueling Method — ***Jongyeon Oh***, *Yongbeom Shin, Dongil Shin*

3:50 Paper 359b: Systematic Chemicals-Based Product Development, Analysis and Chemical Substitution — ***Nichakorn Kuprasertwong***, *Orakotch Padungwatanaroj, Sultana Syeda, Easir A. Khan, Mario Eden, Rafiqul Gani*

4:10 Paper 359c: Computer-Aided Solvent Design for Optimal Selectivity of a Williamson Ether-Synthesis Reaction — ***Lingfeng Gui***, *Alan Armstrong, Amparo Galindo, Fareed Bhasha Sayyed, Stanley P. Kolis, Claire Adjiman*

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(360) Poster Session: Computational Molecular Science and Engineering Forum

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, North Hall E

Jeetain Mittal, Chair
Kayla Sprenger, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

Poster 360a: Exploring canyons in soft and glassy energy landscapes using metadynamics — ***Amruthesh Thirumalaiswamy***, *Robert Riggleman, John C. Crocker*

Poster 360c: The Role of Heteroatom Placement and Chain Branching on Quaternary Ammonium Salts for Phase Transfer Catalysis — ***Brooks Rabideau***, *Rome Parker*

Poster 360d: Investigating the Effect of Oxidic Functional Group on Graphene Oxide-Molybdenum Disulfide Heterostructures As Anode for Sodium-Ion Battery — ***Wonmyung Choi***, *Byungchan Han*

Poster 360e: A Study on the Ionic Conductivity Improvement Mechanism of Halospinel Li2Sc2/3Cl4 By Variable Li and Dopant Concentration — ***SuSeong Hyun***, *Hoje Chun, Minjoon Hong, Byungchan Han*

Poster 360f: Redox Behavior of Single Atom Catalysts for the Upgrading of Plastic Waste-Derived Species — ***Jeremy Hu***, *Eun Mi Kim, Mikyung Hwang, Michael J. Janik, Hilal Ezgi Toraman, Konstantinos Alexopoulos*

Poster 360g: Revisiting Nanoparticle Interactions for Effective Nanofluid Modeling and Simulation — ***Jee-Ching Wang***

Poster 360h: The Molecular Simulation Design Framework (MoSDeF): New Capabilities — ***Co D. Quach***, *Justin Gilmer, Umesh Timalsina, Nicholas C. Craven, Christopher Iacovella, Clare McCabe, Peter Cummings*

Poster 360i: Microbubbles As Non-Invasive Targets for Blood Brain Barrier Disruption: An *in silico* investigation — ***Bailey Zinger***, *Payton Martinez, Kendra Kreienbrink, Mark A. Borden, Kayla Sprenger*

Poster 360j: Deep Reinforcement Learning As a Tool to Enable Coarse Grained Vaccine Models — *Jonathan Faris,* ***Daniel Orbidan***, *Brenden Petersen, Kayla Sprenger*

Poster 360k: Optiboost: A Method for Choosing a Safe and Efficient Boost for the Bond-Boost Method in Accelerated Molecular Dynamics (AMD) Simulations with Hyperdynamics (HD) — ***Jianming Cui***

Poster 360l: Toward Accurate and Transferable Coarse-Grained Peptide Models Using Data-Driven Approaches — ***Luc Christians***, *Alexander J. Pak*

Poster 360m: Predicting Quantum-Accurate DNA Electron Densities and Forces with Equivariant Neural Networks — ***Alex Lee***, *Joshua A. Rackers, William P. Bricker*

Poster 360n: Elucidating Ethylene Hydrogenation on Site Isolated Intermetallic Catalysts — ***Angela Nguyen***, *Griffin A. Canning, Michael J. Janik, Robert Rioux*

Poster 360o: Electron Density Prediction with Graph Neural Networks on Large Catalyst Datasets — ***Ethan Sunshine***, *Muhammed Shuaibi, Zachary Ulissi*

Poster 360p: Exceptional Stability of Gd-Doped UO_2 Against Surface Oxidation: First-Principles Study — ***Minjoon Hong***, *Byungchan Han*

Poster 360q: Explaining Improvements in Li-Ion Battery Performance By Atomic Layer Deposition of Alumina Using Molecular Dynamics Simulation — ***Julie A. Nguyen***, *Abigayle Becker, Krishan Kanhaiya, Alan Weimer, Hendrik Heinz*

Poster 360s: Positive Unlabeled Learning of Peptide Properties — ***Mehrad Ansari***, *Andrew White*

Poster 360t: Elucidating Ligand Selectivity and Partial Agonism Towards Cannabinoid Receptors Using Machine Learning Approaches — ***Soumajit Dutta***, *Balaji Selvam, Austin Weigle, Diwakar Shukla*

Poster 360u: Molecular Simulations of Protein/Ligand-Mediated Microglial Activation in Alzheimer's Disease — ***Emma Lietzke***, *Kimberley Bruce, Kayla Sprenger*

Poster 360v: Coarse-Grained Molecular Dynamics Simulations of ssDNA Loaded Adeno-Associated Virus — ***Tibo Duran***, *Arani Chanda, Willow DiLuzio, Ryan Bellucci, Shivangi Naik, Bodhisattwa Chaudhuri*

Poster 360w: Design of Pore Wall Chemistry to Control Solute Transport and Selectivity — ***Sally Jiao***, *M. Scott Shell*

Poster 360x: Studying Anhydrous Proton Transport on Graphene-Based Materials Using Deep Learning Methods — ***Siddarth Achar***, *Leonardo Bernasconi, Linfeng Zhang, Karl Johnson*

Poster 360y: The Nuclear and Surface Electrostatic Potential As Descriptors of Chemical Interactions — ***Joakim Halldin Stenlid, PhD***, *Frank Abild-Pedersen*

Poster 360z: Understanding DNA Hybridization through Thermodynamics and Kinetics of Abasic Oligomers — ***Mike Jones***, *Brennan Ashwood, Andrei Tokmakoff, Andrew Ferguson*

Poster 360aa: The Chebyshev Interaction Model for Efficient Simulations (ChIMES): Machine-Learned Interatomic Models for Quantum-Accurate Reactive Simulation — ***Rebecca Lindsey***, *C. Huy Pham, Nir Goldman, Laurence E. Fried, Sorin Bastea*

Poster 360ab: Inverse Design of Open Nanocrystal Superlattices Using an Oscillating Pair Potential — ***Chase Petix***, *Michael Howard*

Poster 360ac: Using Text-Mining and Community Knowledge to Quantify and Engineer Stability in MOFs — ***Aditya Nandy***, *Heather Kulik*

Poster 360ad: Electrical Double Layer Capacitance and Polarizability Modeled Using Classical Molecular Dynamics. — ***Bolton Tran***, *Scott T. Milner, Michael J. Janik*

Poster 360ae: Insights of Phenolic Compounds Extraction from an Aqueous Environment Using Natural Deep Eutectic Solvents: Quantum Chemical and Molecular Dynamics Simulation — ***Nikhil Kumar***, *Tamal Banerjee*

Poster 360af: Investigating the Electrocatalytic Reduction of 2,4,6-Tri-Nitro-Toluene (TNT) across Late Transition Metal Surfaces Using Density Functional Theory Methods — ***Andrew Wong***, *Joshua Miller, Brandon Perdue, Michael J. Janik*

Poster 360ag: Identification of Potential TMPRSS2 Inhibitors By Virtual Screening Using Molecular Docking and Machine Learning — ***Suraj Ugrani***

Poster 360ah: Self-Assembly of Lobed Colloidal Particles into Porous Morphologies — ***Brunno C. Rocha***, *Harish Vashisth*

Poster 360ai: Simulation of Lipid Membranes Using Coarse-Grained Model and Reverse-Mapping — ***Hiroya Nitta***, *Taku Ozawa*

Poster 360aj: Determination of Electronic Driving Factor for Selective Adsorption of Arsenic over Phosphorous Oxoanions By Fe(III)-Crosslinked Chitosan Using DFT — ***Obinna Nwokonkwo***, *Christopher Muhich*

Poster 360ak: Insights into the Phase Diagram of Pluronic L64 Using Coarse-Grained Molecular Dynamics Simulations — ***Mangesh Bhendale***, *Arpita Srivastava, Jayant K Singh*

Poster 360am: Understanding the Calcium-Binding Ability of Polystyrene Sulfonate in the Presence of Dodecyl Sulfate By Using Molecular Dynamics Simulations — ***Sonali Gore***, *Kaustubh S. Rane*

Poster 360an: Development and Validation of Non-Bonded Interaction Parameters between Coarse-Grained Amino Acid Models and Water — ***Esmat Mohammadi***, *Soumil Joshi, Sanket Deshmukh*

Poster 360ao: Elucidating the Bulk and Interfacial Structure of Ionic Liquids from the Dilute to Concentrated Regimes Using Molecular Dynamic Simulations — ***Lisa Je***, *Beichen Liu, Matthew Gebbie, Victor Zavala, Reid Van Lehn*

Poster 360ap: Developing Deep Learning Models to Predict Sigma Profiles of Lignin-Derived Organic Molecules — ***Usman Abbas***, *Manh Tien Nguyen, Yuxuan Zhang, Jian Shi, Jin Chen, Qing Shao*

Poster 360aq: Effect of Solvent Quality on Structure and Dynamics of Lignin in Solution — ***Nusrat Jahan***, *Md Masrul Huda, Neeraj Rai*

Poster 360ar: Identifying the Stoichiometry of the Metastable Cu^{3+} State in Alkaline Electrochemical Systems Using DFT-Based Theoretical Raman Standards — ***Lars Ostervold III***, *Bolton Tran, Maxwell Wetherington, Konstantinos Alexopoulos, Lauren F. Greenlee, Michael J. Janik*

Poster 360as: Bayesian Forcefield Driven Monte Carlo and Molecular Dynamics Simulations of O and Cl Promoted Silver Surface Reconstructions — ***Anna Sviripa***, *Ching-Tien Chen, David Flaherty, Christopher Paolucci*

Poster 360at: Explosive Mechanochemistry: Foundations for Strength-Aware Chemical Kinetics — ***Matthew Kroonblawd***, *Brad Steele, Brenden Hamilton, Chunyu Li, Matthew Nelms, Ryan Austin, Laurence E. Fried*

Poster 360au: Protein Interactions Determined from Computational Methods — ***Gregory Dignon***, *Barbara Hribar-Lee, Dima Kozakov, Ken A. Dill*

Poster 360av: A Computational Study for Predicting Stability Differences in Multiple Conformations of the Sars-Cov-2 Frameshifting RNA Element — ***Karim Malekzadeh***, *Gul H. Zerze*

Poster 360aw: Comparison of Advanced Sampling Techniques for Atomistic Scale RNA Folding — ***Kosar Rahimi***, *Gul H. Zerze*

Poster 360ax: Understanding the Normal Bicontinuous Cubic Phase in Gemini Lyotropic Liquid Crystals in Order to Design Selective Separations — ***Nathanael Schwindt***, *Subin Sahu, Douglas L. Gin, Richard D. Noble, Michael Shirts*

Poster 360ay: Parameterization of C, Si, and Ge in the Common Harmonic Form for Molecular Dynamics Simulations — ***Katarina Odak***, *Hendrik Heinz, Alan Weimer*

Poster 360az: The Role of Antiretroviral Therapeutics As Both Inhibitors and Substrates of P-Glycoprotein — ***Daisy Fuchs***, *Sahana Balaji, Kayla Sprenger*

Poster 360ba: Modeling of Photoresist Pattern Formation in EUV Lithography Through Molecular Dynamics Simulations — ***Seungtae Kim***, *Sangwoo Kwon, Won Bo Lee*

Poster 360bb: Benchmarking Martini 3.0 Force Field for Reproducing Thermodynamic Properties of Biomolecular Condensates — ***Ayush Gupta***, *Gul H. Zerze*

Poster 360bc: Understanding Protein Unfolding Under Different Stressors from Molecular Dynamics Simulations — ***Yinhao Jia***, *Janani Sampath*

Poster 360bd: CCR5-Eriously? Reexamining HIV-1 Tropism Switching with *In Silico* directed Evolution — ***Jonathan Faris***, *Bailey Zinger, Brenden Petersen, Kayla Sprenger*

Poster 360be: Monte Carlo Simulations Predicting Adsorption of 1,4-Dioxane in All-Silica Zeolites — ***Samiha Sharlin***, *Tyler R. Josephson*

Poster 360bf: Coarse-Grained Models of Polyetherketoneketone (PEKK) Used to Perform Fusion Weld Simulations and Predict Resulting Mechanical Properties. — ***Chris Jones**, Jenny Fothergill, Rainier Barrett, Eric Jankowski*

Poster 360bg: Investigating Stable and Active Catalysts for Hydrogen Generation Via Methane Pyrolysis in Molten Media, Using *Ab Initio* Molecular Dynamics — ***Ojus Mohan**, Samir H. Mushrif*

Poster 360bh: Extending the MolMod Database to Transferable Force Fields — ***Sebastian Schmitt**, Gajanan Kanagalingam, Daniel Fröscher, Florian Fleckenstein, Hans Hasse, Simon Stephan*

Poster 360bi: Mass Transfer through Vapor-Liquid Interfaces of Binary Mixtures studied by Non-Stationary Molecular Dynamics Simulations — ***Dominik Schaefer**, Jens Staubach, Simon Stephan, Hans Hasse*

Poster 360bj: Theoretical Investigation of The Coverage Effect on Ni-In Intermetallic Catalysts for Selective Hydrogenation of Acetylene to Ethylene — ***Zahra Almisbaa**, Hassan Aljama, Luigi Cavallo, Philippe Sautet*

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(361) Interactive Session: Applied Mathematics and Numerical Analysis

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, North Hall E

Satyajith Amaran, Chair
Kamil Khan, Co-Chair

Sponsored by: Applied Mathematics and Numerical Analysis

Poster 361a: Towards Field Wide Integrated Field Asset Modelling and Associated Optimization Methods — ***Shakeel Ramjanee***

Poster 361b: Towards an Integrated Field Wide Production Optimization Approach — ***Shakeel Ramjanee***

Poster 361c: Mathematical Programming Formulations for the Optimal Generation and Transmission of Electricity in a Macroscopic System Using the Concept of Energy Hub — *Luis R. Barajas-Villarruel, **Vicente Rico-Ramirez***

Poster 361d: Optimal Placement of Portable and Fixed Charging Stations for Electric Vehicles Charging — ***Resmi Suresh, Ayush Bansal***

Poster 361e: Neural-Network Incorporated CFD Models for Adsorption Simulation on Complex Material — ***Zhu Ming***

Poster 361f: Mathematical Modeling of Drug Release from Bi-Layered Polymer Capsules in the Eye — ***Eduardo A. Chacin Ruiz**, Katelyn E. Swindle-Reilly, Ashlee Ford Versypt*

Poster 361g: Differentiating between FSH and HMG Dosage for Personalized Modeling of Superovulation in IVF Patients — ***Bhavi Barnwal**, Urmila Diwekar*

Poster 361i: The Effect of Subdiffusion on the Stability of Autocatalytic Systems — ***Uttam Kumar**, Subramaniam Pushpavanam*

Poster 361j: Extracting Thermodynamic and Fluorescent Properties of Intercalating Dyes from Temperature-Programmed PCR Measurements with Modeling and Optimization — ***Robert DeJaco**, Jacob M. Majikes, Paul N. Patrone, J. Alexander Liddle, Anthony J. Kearsley*

Poster 361k: Prototype Development to Guide the Systemic Description of Biotechnological Processes — ***Priscila Marques Da Paz**, Caroline S. M. Nakama, Galo Carrillo le Roux*

Poster 361l: Predict Transport and Deposition of Multicomponent E-Cigarette Aerosols in a Subject-Specific Airway Model with Different Nicotine Forms: An *in silico* Study — ***Yu Feng**, Ted Sperry*

Poster 361m: A Robust, Multi-Model Model Predictive Control Approach to Vagal Nerve Stimulation of the Human Cardiac System. — ***Oluwasanmi Adeodu**, Yuyu Yao, Michelle Gee, Babak Mahmoudi, Rajanikanth Vadigepalli, Mayuresh Kothare*

Poster 361n: Limits of Entrainment of Circadian Neuronal Networks — ***Georgios Psarellis**, Mihalis Kavousanakis, Michael Henson, Ioannis G. Kevrekidis*

Poster 361o: Modeling and Control of Antibody Purification Via Protein a Affinity Chromatography — ***Fred Ghanem**, Kirti Yenkie, Gerard Capellades, Purnima Kodate*

Poster 361p: Influence of the Spatial Organization of Contaminants on Bioremediation — ***Jenna Ott**, Yaxin Duan, Daniel Amchin, Sujit Datta*

Poster 361q: Energy optimization of chemical process : Comparison of derivative-free algorithms — ***Minsu Kim**, Areum Han, Jaewon Lee, Jinwoo Park, Jonggeol Na, Il Moon*

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(362) Interactive Session: Data and Information Systems

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, North Hall E

Joseph Kwon, Chair
Stevan Dubljevic, Co-Chair
Yifu Chen, Co-Chair
Junyao Xie, Co-Chair

Sponsored by: Information Management and Intelligent Systems

Poster 362a: A Reinforcement Learning Approach for Stochastic Cutting Stock Problem — ***Jie-Ying Su**, Jia-Lin Kang, Shi-Shang Jang*

Poster 362b: Multi-objective Optimization of Process Efficiency and CO2 Emission for On-Site Hydrogen Production Process Using Hybrid Data-Driven Model. — ***Jaewon Lee**, Seokyoung Hong, Hyungtae Cho, Seongbin Ga, Junghwan Kim*

Poster 362c: Data-Driven Surrogates with Physics-Informed Architecture for Modelling Non-Linear Stiff Dynamic Systems — ***Suryateja Ravutla**, William Bradley, Fani Boukouvala*

Poster 362e: A Comparative Evaluation of Machine Learning Algorithms in Predicting Syngas Fermentation Outcomes Using Limited Experimental Data — ***Garrett W. Roell**, Ashik Sathish, Ni Wan, Zhiyou Wen, Yinjie Tang, Forrest Sheng Bao*

Poster 362f: Development of Bayesian Machine Learning Algorithms for Optimal Nonlinear Model Selection and Parameter Estimation from Noisy Data of Unknown Characteristics — ***Samuel Adeyemo**, Debangsu Bhattacharyya*

Poster 362g: Soft Actor-Critic Deep Reinforcement Learning with Hybrid Actions for Scheduling of Energy Systems Under Demand Response — ***Gustavo Campos**, Nael El-Farra, Ahmet Palazoglu*

Poster 362h: Physics Informed Machine Learning for Feasibility Analysis — ***Zachary Kilwein**, Michael Eydenberg, Logan Blakely, Fani Boukouvala*

Poster 362i: Virtual Sample Generation Based on Quantile Regression Variational Generative Adversarial Network for Soft-Sensing Modeling — *Xiaohan Zhang, Qunxiong Zhu, **Xunyuan Yin***

Poster 362j: Rnn and Transfer Learning for Battery Life Prediction of Electric Vehicles Based on Real-Road Driving Obd Data and Lab Measurements — ***Juri Lim**, Dongil Shin, DongKuk Jang, Jaewook Lee*

Poster 362k: Accurate Surrogate Models for Stochastic Simulations Using Parin: Parameter As Input-Variable — ***Samira Mohammadi**, Selen Cremaschi*

Poster 362l: Cost Optimization of Steel Alloying Elements with Machine Learning Based Jominy Hardness Profile Prediction — ***Louis Allen**, Peyman Z. Moghadam, Joan Cordiner*

Poster 362m: Hybrid, Interpretable Machine Learning for Thermodynamic Property Estimation Using Grammar2vec for Molecular Representation — ***Vipul Mann***, *Karoline Brito, Rafiqul Gani, Venkat Venkatasubramanian*

Poster 362n: Predicting Activity Coefficients at Infinite Dilution Using Hybrid Residual Graph Neural Networks — ***Edgar Ivan Sanchez Medina***, *Steffen Linke, Martin Stoll, Kai Sundmacher*

Poster 362o: Improved Performance of Artificial Neural Networks Via Hyperparameter Optimization and Data Augmentation for a Small Number of Data Sets — ***Pyeong-Gon Jung***, *Young-Il Lim*

Poster 362p: Data-Driven Modeling of Complex Nonlinear Systems Using Hybrid Series and Parallel Nonlinear Static – Dynamic Stochastic Neural Networks — ***Angan Mukherjee***, *Debangsu Bhattacharyya*

Poster 362q: Multi-Rate Data-Driven Models for Lactic Acid Fermentation - Parameter Identification and Prediction — ***Satish Parulekar***, *Jingwei Gan*

Poster 362r: Modeling Dynamics of Material Flows in Coupled Industrial Processes Using Data Driven System Identification — ***William Farlessyost***, *Shweta Singh*

Poster 362s: Developing Risk Assessment Framework for Wildfire in the United States – a Deep Learning Approach — ***Pingfan Hu, Zhuoran Zhang***, *Qingsheng Wang*

Poster 362u: High-Throughput Screening for Identifying Potential Chemical Exposure Scenarios at End-of-Life Stage — *Jose Hernandez-Betancur, Gerardo Ruiz-Mercado,* ***Mariano Martin***

Poster 362v: Experimental Evaluation of the Level Detection in Separators Using Electrical Tomography — *Antti Nissinen, Arto Voutilainen,* ***Pekka Kaunisto***, *Jonathan Vänskä, Mika Tienhaara*

Poster 362w: Cover Cut Based Algorithm for Optimal Sensor Network Design — ***Arjun M***, *Nabil Magbool Jan*

Poster 362x: Ensemble Learning for Fault Diagnosis in Chemical Processes: Fusion of Results through a K-Nearest Neighbors Algorithm — ***Bairi Sai Vasista, Rajagopalan Srinivasan***

Poster 362y: Failure Stage Classification and Its Application to Predicting Remaining Useful Life of Bearings — ***Bahareh Hassani***, *Q. Peter He*

Poster 362z: Root Cause Identification Using Cross-Correlation Weighted Lag in Chemical Plants — ***Abhishek Bansal***, *Navadha Mankodi, Mohd Faheem Ullah, Resmi Suresh, Raghunathan Rengaswamy*

Poster 362aa: Process Monitoring and Online Fault Detection and Diagnosis Using Deep Recurrent Neural Networks on Plant Data — ***Lucky E. Yerimah***, *Sambit Ghosh, Yajun Wang, Yanan Cao, Jesus Flores-Cerrillo, B Wayne Bequette*

Poster 362ab: Digitalization of an Experimental Electrochemical Reactor Via the Smart Manufacturing Innovation Platform — ***Berkay Citmaci***, *Junwei Luo, Prakashan Korambath, Joonbaek Jang, Carlos Morales-Guio, Jim Davis, Panagiotis Christofides*

Poster 362ac: Physics-Based Penalization for Hyperparameter Optimization in Gaussian Process Regression — ***Jinhyeun Kim***, *Kamran Paynabar, Christopher O. Luettgen, Fani Boukouvala*

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(363) Interactive Session: Systems and Process Control

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, North Hall E

Fernando V. Lima, Chair
Ali Mesbah, Co-Chair

Sponsored by: Systems and Process Control

Poster 363a: Cost-Optimal Multi-Effect Mechanical Vapor Recompression Evaporation Configuration in Pulp and Paper Industry — ***Yurim Kim***, *Deok Ju Kim, Jonghun Lim, Hyungtae Cho, Junghwan Kim*

Poster 363b: Molten-Metal Bubble Column Reactor Design to Produce Hydrogen Using a Combination of Catalytic and Non-Catalytic Kinetic Models — ***Bang Thanh Le***, *Young-Il Lim, Son Ich Ngo, Uen-Do Lee, Youn-Bae Kang*

Poster 363c: Process Operability Mapping Using Neural Networks — ***Karan Waghela***, *Victor Alves, John Kitchin, Fernando V. Lima*

Poster 363d: Selection of Self-Optimizing Controlled Variables Using Principal Component Analysis — *Sunil Kumar,* ***Nabil Magbool Jan***

Poster 363e: A Data-Driven Dynamic Modeling Methodology Based on POD/Oed/ANNs Method for Large-Scale Dynamic Systems — ***Weiguo Xie***

Poster 363f: Machine Learning and System Identification for Dynamical Systems: A Comparative Review — ***Akhil Ahmed***, *Antonio del Rio Chanona, Mehmet Mercangoez*

Poster 363g: Data Driven Discovery of Chemical Reaction Kinetics — ***Md Rizwan***, *David Eklund, Ronnie Andersson*

Poster 363h: Comparing Reinforcement Learning and Bayesian Optimization for Tuning MPC Policies — ***David Pérez-Piñeiro***, *Sigurd Skogestad*

Poster 363i: CFD Modeling of Gravity Separator with PID Interface Controller — ***Chang Kai Wu***, *Eugene Yan, Mike Ma, Hossam Metwally, Sravan Nallamothu*

Poster 363j: Modelling of Fluid Flow and Mass Transfer in a Multi-Channel Microfluidic Reactor Using Computational Fluid Dynamics. — ***Oluwaseyi Ayeni***, *Holly A. Stretz*

Poster 363k: Multiscale Modeling and Control of Spray Coating of Quantum Dots — ***Niranjan Sitapure***, *Joseph Kwon*

Poster 363l: Matrix Non-Structural Model and Its Application in Heat Exchanger Network without Split Streams — ***Ding Hao Li***, *Jingde Wang, Wei Sun*

Poster 363m: Continuous and Discrete Control of Flow Networks — ***Varghese Kurian***, *Sajay Velmurugan, Sridharakumar Narasimhan*

Poster 363o: Nonlinear Model Predictive Control for the Dividing Wall Column — ***Xing Qian***, *Shengkun Jia, Lorenz Biegler*

Poster 363p: Effects of Electromagnetic Fields on Initial Bubble Size of CH_4 – Sn Molten Metal Based Bubble Column Reactor Using a Volume of Fluid CFD Model — ***Hanh Bui***, *Son Ich Ngo, Young-Il Lim*

Poster 363q: Model Predictive Control Considering Stochastic Heat Generation for Thermal Management of Electric Vehicle — ***Hyein Jung***, *Changbeom Hong, Hyeonwoo Cho, Se-Kyu Oh, Yeonsoo Kim, Jong Min Lee*

Poster 363t: Data-Gathering Lyapunov-Based Economic Model Predictive Control: Considering Interpretability and Physics-Based Model Selection — ***Henrique Oyama***, *Fnu Akkarakaran Francis Leonard, Rebecca Lopez, Dominic Messina, Helen Durand*

Poster 363u: Tuning MPC through System-Level Parameterization and Inverse Optimization — ***Wentao Tang***

Poster 363v: Online Impedance Analysis Using Chirp Signals in Linear and Non-Linear Systems — ***Rigved Samant***, *Resmi Suresh, Raghunathan Rengaswamy*

Poster 363w: A New MILP Formulation for Scheduling Cleaning in Heat Exchanger Networks Consisting of Multi-Pass Heat Exchangers — ***Parag Patil, Babji Srinivasan, Rajagopalan Srinivasan***

Poster 363x: Directed Randomization to Detect for Cyberattacks on Nonlinear Systems Under Lyapunov-Based Economic Model Predictive Control — ***Keshav Kasturi Rangan***, *Kip Nieman, Fnu Akkarakaran Francis Leonard, Helen Durand*

Poster 363y: Pipelines Multi-Product Scheduling and Delivering By Model Predictive Control — ***Lu Zhang***, *Stevan Dubljevic*

Poster 363z: Constraint-Dropping in Cutting-Set Based Robust Optimization: Enabling Robust Heat Pump Allocation — ***Tom Savage***, *Dongda Zhang, Antonio del Rio Chanona*

Poster 363aa: Modeling and Predictive Control of the Coffee-Ring Effect in Coalescing QD-Droplets — ***Omkar Newalkar***, *Niranjan Sitapure, Joseph Kwon*

Poster 363ab: Operator's Eye Gaze Analytics for Evaluating Usability of Human Machine Interfaces in Process Control Applications — ***Mohammed Aatif Shahab***, ***Babji Srinivasan***, ***Rajagopalan Srinivasan***

Poster 363ac: Data-Driven ARX Models with Measurable Disturbances for Model Predictive Control (MPC) of Crop Irrigation — ***Jisung Jang***, *Q. Peter He*

Poster 363ad: Adaptive Economic Model Predictive Control for Batch Processes: Application to Rotational Molding Process — ***Aswin Chandrasekar***, *Hassan Abdulhussain, Vladimir Gritsichine, Michael R. Thompson, Prashant Mhaskar*

Poster 363ae: Online Data-Driven Closed-Loop Model Predictive Control of Nonlinear Systems Using Artificial Neural Networks — ***Andrew Branen***, *Mayuresh Kothare, Gautam Kumar*

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(364) Interactive Session: Systems and Process Design

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, North Hall E

Matthew Realff, Chair

Sponsored by: Systems and Process Design

Poster 364a: Modeling and Analysis of the Production of Formaldehyde from Methanol — ***Omar Almaraz***, *Md Emdadul Haque, Srinivas Palanki*

Poster 364b: Towards an Integrate Field Wide Production Optimization Approach for Upstream Field Recovery — ***Shakeel Ramjanee***

Poster 364c: A Mass Integration Model between Hydraulic Fracturing Processes and a Power Plant — *Moises Ferreyra-Quiroz,* ***Luis Lira-Barragan***, *José María Ponce-Ortega*

Poster 364d: Comparing Formulations for Global Flowsheet Optimization with Simultaneous Heat Integration — *Steffen Fahr, Alexander Mitsos,* ***Dominik Bongartz***

Poster 364e: Optimizing Resilience in the Assessment of the Water-Energy-Food Nexus — ***Jesus Manuel Nuñez Lopez***, *Eusiel Rubio-Castro, Jose Ponce-Ortega*

Poster 364f: Finite Element Refinement and Selection on the Integration of Design and Control: A Hamiltonian Function-Profile-Based Approach. — ***Oscar Palma-Flores***, *Luis Ricardez-Sandoval*

Poster 364g: Profit Distribution in Interplant Heat Integration Using a Hybrid Optimization Approach — ***Francisco Javier López Flores Sr.***, ***Luis Fernando Lira-Barragán III***, *Luis Germán Hernández-Pérez, Eusiel Rubio-Castro, Jose Ponce-Ortega*

Poster 364h: Solvent Mixture Design Using COSMO-RS Descriptors and Molecular Simulations — ***Jianping Li***, *Christos Maravelias, Reid Van Lehn*

Poster 364i: Development of a Resilience Model for the Analysis of Process Systems at the Early Design Stage — ***Joan Cordiner***, *Freya Vesey*

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(365) Interactive Session: Systems and Process Operations

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, North Hall E

Dimitrios Georgis, Chair
Qi Zhang, Co-Chair

Sponsored by: Systems and Process Operations

Poster 365a: Feedback State-Space Mapping Framework for Dynamic Operability Analysis — ***San Dinh***, *Fernando V. Lima*

Poster 365b: Mixed-Integer Adjustable Robust Optimization Under Exogenous Uncertainty — ***Byungjun Lee***, *Styliani Avraamidou*

Poster 365c: Towards an Integrated Field Wide Production Optimization Approach for Upstream Hydrocarbon Recovery — ***Shakeel Ramjanee***

Poster 365d: New and Efficient Interval Sampling Method for Use of P-Boxes in Off-Line Quality Control — ***Urmila Diwekar***, *Mark A. Stadtherr*

Poster 365f: A Reinforcement Learning Approach for Optimal Scheduling of Multiproduct Batch Plants — *Prasoon Gupta,* ***Nabil Magbool Jan***

Poster 365g: Development of Artificial Intelligence Based Models for Biomass Gasification — ***Satish Parulekar***, *Essa Almutar*

Poster 365h: System-Wide Anomaly Detection By Single Value Using Mscred in MEG Regeneration Pilot Plant — ***Nayoung Lee***, *Hyunho Kim, Jinkwan Jang, Yutaek Seo*

Poster 365i: Multiperiod Generalized Disjunctive Programming Optimization in Idaes: Simultaneous Design and Operation of an Integrated Energy System — ***Edna Rawlings***, *Jaffer Ghouse, Naresh Susarla, John Siirola, David Miller*

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(366) Poster Session: Chemical Engineering Education

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, North Hall E

Monica Lamm, Chair
J. Patrick Abulencia, Co-Chair

Sponsored by: Education

Poster 366l: Ocular Drug Delivery and Unsteady-State Mass Transfer: A Project-Based Learning Approach Using Comsol Multiphysics — ***Daniel Lepek***

STUDENT LEARNING AND ASSESSMENT

Poster 366a: Gamification of Learning: Designing a Safety Assessment Card Game — ***Seng Hoe (billy) Hue***, *Elton M. Dias*

Poster 366b: The Oral Exam – an Alternative Approach to Assessment — ***J. Patrick Abulencia***

Poster 366c: Data-Driven Analysis of Learning Behavior within a Student-Led Chemical Engineering Wiki — ***Thomas Nok Hin Cheng***, *Luc Paoli, Samuel Chun-Hei Lam, David -, Pierre Walker, Jerry Y. Y. Heng, Marsha Maraj*

EDUCATIONAL TOOL DEVELOPMENT

Poster 366d: Making Unit Operations an Immersive Experience through Augmented Reality — ***Jacob Crislip***, *Esai Lopez, Cameron Armstrong, Andrew R Teixeira*

BROADENING PARTICIPATION

Poster 366e: Translating DNA Origami Nanotechnology to Middle School, High School, and Undergraduate Laboratories — ***Anjelica Kucinic***, *Peter Beshay, Patrick Halley, Carlos E. Castro, Michael Hudoba*

Poster 366f: Sense of Belonging within Chemical Engineering and Its Impacts upon Retention — ***Duncan Mullins***

Poster 366g: Graduate Involvement in Vertically Integrated Projects for Biomaterials Education Research — ***Alec Svenson***, *Jennifer Weiser*

Poster 366h: Increase Recycle to Reduce the Purge – a System to Improve Curriculum Retention — ***John Wagner***, *Amanda P. Malefyt, Arthur Hersel, Jacob R. Borden*

Poster 366i: Developing a Framework to Examine Women STEM Faculty's Participation in Entrepreneurship Education Programs — ***Aida López Ruiz***, *Prateek Shekhar, Jacqueline Handley, Aileen Huang-Saad*

Poster 366j: Self-Efficacy in First-Year STEM Majors Correlates with Academic Progression — *Robert Petrulis, Sona Gholezadeh,* ***Edward Gatzke***

TRANSPORT AND MODELING

Poster 366k: Using Matlab, Simulink, and Simscape in Chemical Engineering Fluid Mechanics Courses — ***Aycan Hacioglu***, *Terry Denery, Bradley Horton*

LABORATORY COURSES

Poster 366m: Development of 3D Printed Desktop Learning Module for Learning Packed and Fluidized Bed Concepts — ***Zeynep Durak***, *Bernard Van Wie, David B. Thiessen*

Poster 366n: A Hands-on Experience to Study Membrane Technology Developed By Undergraduate Chemical Engineering Students — ***Andie Veeder***, *Jackqueline Steinman-Ptacek, Natacha Souto-Melgar*

(367) Poster Session: Thermodynamics and Transport Properties (Area 1A)

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, North Hall E

Diwakar Shukla, Chair
Andrew Paluch, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

Poster 367a: Evaluation of Vapor-Liquid and Solid-Liquid Equilibria for Systems Containing Tetrahydrofuran and Dimethyl Carbonate Using Asog Model — ***Katsumi Tochigi***, *Hiroyuki Matsuda, Kiyofumi Kurihara*

Poster 367b: A Note on Selectivity of Co-Solvent for Drug Production Process Using Ternary Infinite Dilution Activity Coefficient –Etodolac + Water + Co-Solvent System – — ***Katsumi Tochigi***, *Hiroyuki Matsuda, Kiyofumi Kurihara*

Poster 367c: Enthalpy of Mixing and Liquid Structure of Primary and Secondary Alcohols — ***Chun-Kai Chang***, *Joern Siepmann*

Poster 367d: Volumetric and Acoustic Properties of Saccharides in Aqueous Solutions Containing Polyethylene Glycols (PEGs) — *P J. Castro,* ***Ricardo Torres***

Poster 367e: Sustainable Methane Storage Using Gas Hydrates with Superabsorbent Polymers (SAPs) and Tetrahydrofuran (THF) Under a Quiescent System — ***Dong Woo Kang***, *Wonhyeong Lee, Yun-Ho Ahn, Jae Lee*

Poster 367f: Thermodynamics Modeling Employing the Compound Energy Formalism with Novel Complementary Use of Experimental and First Principles Data: A Case Study of $Ba_{1-x}Sr_xFeO_{3-\delta}$ — ***Steven Wilson***, *Ellen B. Stechel, Christopher L. Muhich*

Poster 367g: Effect of Cationic Species on the Activity and Inhibition Performance of NO_2^-/NO_3^- Corrosion Inhibitors — ***Ahmed Mohamed***, *Donald Visco Jr., David M. Bastidas*

Poster 367h: Development of the Hydrocarbon Polymer Electrolyte Membranes and the Modeling Analysis By Using Molecular Dynamics — ***Hyunseo Park***, *Hyoje Son, Sweety Verma, Pil Seung Chung*

Poster 367i: Modifying Reactor Structure to Improve Efficiency from a Heterogeneous Approach — ***Kei Sakurai***, *Feng Xu, Yuki Sato, Yuka Sakai, Yasuki Kansha*

Poster 367j: Study of Granular Flow in a Wedge-Shaped Hopper Using DEM Simulations — ***Afroz Momin Sr.***

Poster 367k: Rheological Characteristics of Tetra-n-Butylammonium Bromide Hydrate As a Thermal Energy Carrier — *Hyunho Kim, Junjie Zheng,* ***Ponnivalavan Babu***, *Praveen Linga*

(368) Poster Session: Nanoscale Science and Engineering Forum

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, North Hall E

Yoonjee Park, Chair
Reginald Rogers Jr., Co-Chair

Sponsored by: Nanoscale Science and Engineering Forum

Poster 368a: Surface-Mediated Assembly of Site-Modified Green Fluorescent Protein into Two-Dimensional Nanosheets As a Platform for Hierarchical Materials Fabrication — ***Nada Naser***, *Karthik S. Pushpavanam, Jinrong Ma, François Baneyx*

Poster 368b: A Machine Learning Study on the Result of Polarizable Molecular Dynamics of Ionic Liquid-Based Solid Polymer Electrolytes for Li^+-Ion Batteries By Graph Dynamical Networks — ***Chanui Park***, *Anseong Park, Sebin Kim, Seunghyok Rho, Minhwan Lee, Sangwoo Kwon, JunBeom Cho, Seulwoo Kim, Won Bo Lee*

Poster 368c: Lithium Ion Transport Mechanism in PYR_{14}tfsi/PEO Branched Nanopore System: A Polarizable Molecular Dynamics Study — ***Sebin Kim***, *Seulwoo Kim, Minhwan Lee, Chanui Park, Anseong Park, Sangwoo Kwon, JunBeom Cho, Seunghyok Rho, Won Bo Lee*

Poster 368d: Improvement of Storage Stability of mRNA Vaccine Using Lipid Based Drug Delivery System — *MinJeong Kim, Taekyoung Lee, Hyunjin Kim, Sangmin Lee,* ***Minsub Chung***

Poster 368e: Synthesis of Metal-Organic Frameworks (MOFs) and Evaluation of Their Toxicological Profiles. — ***Olivia Rose***, *Yon Rojanasakul, Cerasela Zoica Dinu*

Poster 368f: Diffusion Growth Mechanism of Penta-Twinned Ag/Cu Nanowires: Multiscale Theory — ***Jianming Cui***

Poster 368g: Protein Templated Core/Shell Nanostructures for Photothermal Therapy and SERS Mediated Intracellular ROS Detection — ***Animesh Pan***, *Muzahidul Islam Anik, Md Golam Jakaria, Samantha Meenach, Geoffrey D. Bothun*

Poster 368h: Optimizing Composition and Solar Light Conditions for the Reversible Diels-Alder Reaction in Titanium Nitride Nanoparticle-Laden Epoxy — ***Madeline Finale, Kavon Mojtabai, Arnob Dipta Saha, Sanchari Chowdhury***

Poster 368i: Synthesis of Near-Infrared Pigments for Novel Sensor Applications — ***John Clark***, *Holly A. Stretz, Agoston Kiss*

(369) Poster Session: NSEF Graduate Student Poster Competition

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, North Hall E

Yoonjee Park, Chair
Reginald Rogers Jr., Co-Chair

Sponsored by: Nanoscale Science and Engineering Forum

Poster 369a: Upgrading Food Waste to High Commercial Value Chemicals — ***Yagya Gupta***, *Laura Elizabeth Beckett, Sunitha Sadula, Vibin Vargheese, LaShanda Korley, Dionisios Vlachos*

Poster 369b: Controlling Metal Nanoparticle Size Distribution through Microreactor Residence Time Distribution — ***Faiz Khan***, *Jessica Winter*

Poster 369c: Development and Characterization of Recyclable Epoxy/Refractory Plasmonic Nanoparticles for Additive Manufacturing — ***Arnob Dipta Saha***, *Kavon Mojtabai, Madeline Finale, Samantha Lindholm, Brandon McReynolds, Youngmin Lee, John McCoy, Sanchari Chowdhury*

Poster 369d: Development of Magnetic Nanoparticles and Nanocomposites for Environmental and Biomedical Applications — ***Pranto Paul***, *J. Zach Hilt*

Poster 369f: Development of Methods for Precise, Multifactor Tuning of Shell Morphology on Silica-Encapsulated Gold Core-Shell Nanoparticles — ***Ellis Hammond-Pereira***, *Zengran Sun, Steven Saunders*

Poster 369g: NSEF Poster Session: Computational Studies on the Structural Properties of Square Colloids with Offset Magnetic Dipoles — ***Matthew Dorsey***, *Orlin D. Velev, Carol Hall*

(370) Poster Session: Bioseparations

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, North Hall E

Piran Kidambi, Chair
Heather Chenette, Co-Chair

Sponsored by: Bio Separations

Poster 370b: Demonstrating the Scale up of Single-Use Centrifugation/Washing/Media Exchange for Cell Cultures at the Bench, Pilot Plant and Manufacturing Bioreactors. — ***David Richardson Sr.***

(371) Poster Session: Fundamentals and Applications of Adsorption and Ion Exchange

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, North Hall E

Masoud Jahandar Lashaki, Chair
Reza Haghpanah, Co-Chair

Sponsored by: Adsorption and Ion Exchange

GAS-PHASE APPLICATIONS OF ADSORPTION

Poster 371a: Guide to COF Adsorbent for Ammonia-based Green Hydrogen with Multi-scale Evaluation Approach — ***Nahyeon An****, Seongbin Ga, Giyeol Lee, Hyungtae Cho, Junghwan Kim*

Poster 371b: Amine-Modified Silica Materials for Direct Carbon Dioxide Capture from the Atmosphere — ***Amirjavad Ahmadian Hosseini****, Masoud Jahandar Lashaki*

Poster 371c: Adsorption Mechanism of Ultra-Low Concentration H_2s and THT in CH_4 on Zeolites in the Presence of CO_2 — *Young-Ho Cho,* ***Gina Bang****, Chang-Ha Lee*

Poster 371d: A New Dynamic Vapor Sorption Instrument for the Investigation of Water Sorption on Porous Materials — ***Thomas Paschke****, Frieder Dreisbach, Volodymyr Bon*

Poster 371e: Adsorption Equilibria and Kinetics of CO_2, CO, CH_4, N_2, O_2, and H_2 on Silica-Based Adsorbents — *Jiwon Jung, Hongjoo Do, Kyounghee Chung,* ***Jun-Ho Kang****, Moonkyung Cho, Chang-Ha Lee*

Poster 371f: Performance Evaluation and Comparison of Conventional and Emerging Adsorbents in Their Applications to a CO_2 Capture Vacuum Pressure Swing Adsorption (VPSA) Process — ***Yixuan Zhang****, Hyungwoong Ahn*

Poster 371g: Adsorbents for Selective Adsorption of VOC Biomarkers from Simulated Breath — ***Ojuolape Oghenetega****, Krista Walton*

Poster 371h: Epoxide-Modified Amine-Based CO_2 Adsorbent for Direct Air Capture — ***Yao Ma****, Joo-Youp Lee*

Poster : Boosting Volumetric and Gravimetric H2 Storage Capacity of Carbon-Based Sorbents Through Tuning Surface Chemistry and Densification Approaches — ***Ruthra Murugavel****, Fateme Rezaei*

ADSORBENT MATERIALS

Poster 371j: Porous Carbon from Non-Recyclable Plastic Wastes — *Dipendu Saha,* ***Brian Hoffman****, Joanna Weyrich, Garret Gallo*

Poster 371k: Direct Ink 3D Printing of Porous Carbons — ***Marisa Comroe****, Dipendu Saha*

Poster 371l: Diffusion Studies of Hydrocarbons in Ill-Crystallized or Desilicated ZSM-5 Catalysts — *João Victor S. Cardoso, Laura Silva, Leandro Martins, Francisco Murilo Tavares de Luna,* ***Celio Cavalcante Jr.***

Poster 371m: Understanding Fluid Phase Behavior in Geometrically Disordered Mesoporous Materials — ***Henry R. N. B. Enninful***

Poster 371r: Boosting Volumetric and Gravimetric H_2 Storage Capacity of Carbon-Based Sorbents Through Tuning Surface Chemistry and Densification Approaches — ***Ruthradharshini Murugavel****, Fateme Rezaei*

LIQUID-PHASE APPLICATIONS OF ADSORPTION

Poster 371o: Synthesis of Mussel-Inspired Polydopamine Mediated with Ionic Liquid As a Sustainable Adsorbent for the Selective Removal of Anionic Pollutants for Wastewater Applications — *Rawan Abu Alwan,* ***Botagoz Zhuman****, Mahendra Kumar, Hassan Arafat, Enas Al Nashef*

Poster 371p: Investigating Alkali-Activated Fly Ash Based Materials As Adsorbents for Heavy Metal Sorption — ***Monday Okoronkwo****, Sukanta K. Mondal*

Poster 339c: Hyper-Crosslinked Tetraphenylboron (TPBx) As a Versatile Platform Material for the Development of Sorbents for Various Metal Ions — ***Grace Nisola****, John Edward Sio, Khino Parohinog, Hern Kim, Erwin Escobar, Wook-Jin Chung*

Poster 143d: Phosphorous-Doped Mesoporous Carbon As an Efficient Adsorbent for the Recovery of Neodymium (III) Metal Ion from an Aqueous Medium — ***Gebremedhn T. Gebremichael****, Hiluf Tekle Fissaha, Grace Nisola, Wook-Jin Chung*

Poster 371q: Demonstration of Iodine Removal Efficiency of MOF-Based Sorbents from Nuclear Waste Solutions in the Presence of Interfering Ions — ***Turki Alghamdi****, Ali Rownaghi, Fateme Rezaei*

(372) Poster Session: General Topics on Separations

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, North Hall E

Joshua Thompson, Chair
Stephen Ritchie, Co-Chair

Sponsored by: General Topics and Other Methods

Poster 372b: Hybrid Heat-Integrated Design Alternatives of Dimethyl Carbonate Reactive Distillation — ***Minyong Lee****, Heecheon Lee, Chaeyeong Seo, Jeongwoo Lee, Jae Lee*

Poster 372c: A Low-Temperature Hollow Fiber Membrane Reactor for Propane Dehydrogenation — ***Lu Liu****, Antara Bhowmick, Dongxia Liu, Chen Zhang*

Poster 372d: The Technology Development in Magnesium Production and Separation — ***Lucas Arndt****, Weiguo Xie, Richard Davis*

Poster 372e: Selective Recovery of Au^{3+} *via* Complexation-Reduction Capture and Release By Thermo-Responsive P(NIPAM-co-15TCE-4)@SiO_2 Nanoparticles. — ***Hiluf Tekle Fissaha****, Grace Nisola, Wook-Jin Chung*

Poster 372g: $Co_{1-x}[Fe(III)(CN)_6]$/Ag for Electrochemical Recovery of Cobalt Ion from Spent Nickel Metal Hydride Batteries — ***Hana G. Zeweldi****, Gebremedhn T. Gebremichael, Negasi Teklay Weldesemat, Grace Nisola, Wook-Jin Chung*

Poster 372i: Selective Adsorption of Chlorofluorocarbons (CFC) and Hydrochlorofluorocarbons (HCFC) in Hydrofluorocarbon's (HFC) Using Adsorbent Supported Metal Oxide. — ***Anup Kumar Doraiswamy***

Poster 372j: Project Earth (Environmentally Applied Research Towards Hydrofluorocarbons) Ionic Liquids Approach — ***Kalin R. Baca****, Greta M. Olsen, Lucia Matamoros Valenciano, Madelyn Bennett, Dorothy M. Haggard, Mark B. Shiflett*

Poster 372k: Impact of Wafer Chemistry on Electrodeionization Removal and Selectivity — ***Leticia Santos de Souza****, Jamie Hestekin, Christa N. Hestekin*

Poster 372l: Estimation of Supersaturation in Pressure-Driven Supersaturated Gas-Liquid Systems — ***Sushobhan Pradhan****, Prem Bikkina*

Poster 372m: Identification of the Innovative Separation Technique for Sustainable Society — ***Akanksha Prasad****, Dr. Utkarsh Maheshwari*

Poster 372o: Understanding Separation Mechanisms of Monoatomic Gases, Such As Kr and Xe, Via DD3R Zeolite Membrane Using Molecular Dynamics — ***Bandar Bashmmakh****, Xiaoyu Wang, Cynthia J. Jameson, Sohail Murad*

Poster 372p: Phase Equilibria for HFC-32, HFC-125, and Binary Mixtures (R-410A) with a Variety of Ionic Liquids — ***Kalin R. Baca***, *Greta M. Olsen, Lucia Matamoros Valenciano, Madelyn Bennett, Dorothy M. Haggard, Mark B. Shiflett, Mark B. Shiflett*

Poster 372q: Separation of Dispersed Water from ULSD Using a Wire Mesh Electrowet Coalescer — ***Mohammad Assaleh***, *George G. Chase*

Poster 372r: Barriers to Electrodialysis Implementation: Maldistribution and Its Impact on Resistance and Limiting Current Density — ***Jack Ledingham***, *Kyra Sedransk Campbell, Ben In 't Veen, Lucas Keyzer, Alasdair Campbell*

Poster 372s: Utilizing Capillary Isoelectric Focusing to Identify Uremic Toxins in the Urine of Chronic Kidney Disease Patients — ***Haley Duncan***, *Christa N. Hestekin*

Poster 372t: Porous Ionic Liquids: Theoretical and Experimental Research — ***Hongping Li***

Poster 372u: Eutectic Ionic Liquids for Efficient Gas Separation — ***Guokai Cui***

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(373) Poster Session: Membrane Separations

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, North Hall E

William Phillip, Chair
Christine Duval, Co-Chair

Sponsored by: Membrane-Based Separations

LIQUID PHASE SEPARATIONS

Poster 373a: Designing, Preparing and Characterizing Alkali Treated Graphitic Carbon Nitride Thin Film Composites (TFC) Membranes for Efficient Dye Salty Water Separation. — ***Ameya Tandel***, *Haiqing Lin*

Poster 373b: Membrane Material Development for Spaceflight Wastewater Applications — *Mary Lind,* ***Elisabeth Thomas***

Poster 373c: Effect of Ionic Liquid Cations and Anions on the Cellulose Acetate Membrane Characteristics and Performance for Water Treatment — ***Atta Ur Razzaq***, *Milad Esfahani, Jason Bara*

Poster 373d: 2D Assembly of Graphene Oxide Nanoribbon *Via* Slot-Die Coating and Its Application for Organic Solvent Nanofiltration — *Dae Woo Kim,* ***Ji Hoon Kim***

Poster 373f: Microwave-Assisted Nanoporous Multilayer Graphene Membrane with Ultrafast Organic Solvent Nanofiltration — ***Junhyeok Kang***, *Dae Woo Kim*

Poster 373g: Treatment of Produced Water Using Sand Filtration and Ultrafiltration Using Modified α-Alumina Membranes — ***Anirban Ghosh***, *Diako Mahmodi, Michael Miranda, Clint Aichele, Seokjhin Kim*

Poster 373h: Production of Nanofiber Membranes Using Centrifugal Spinning — *Divine Kavunga, Beck Bruch, Cory Stone,* ***Maryam Amouamouha***, *Travis Walker*

Poster 373i: Ceramic Membrane Synthesis, Application and Characterization — ***Tejay Lanjewar Sr.***, *Mahesh Varma*

Poster 373k: Progress in the Development of Membranes for Pressure Retarded Osmosis Process — ***Dr. Syed Zaidi***, *Haleema Saleem Sr.*

Poster 373l: Separation of Olefin-Paraffin Mixtures with Optiperm^{TM} customized Amorphous Fluoropolymer Membranes — ***William Charlton***, *Christine Parrish, Ken Loprete, Marissa Bonanno, Sudip Majumdar*

Poster 373j: Implications of Shear and Cation Choice on Dynamics of Nonliving Natural Organic Matter — ***Kathlyn Mealio***, *Holly A. Stretz, Martha J. M. Wells, Katherine Slamen, John Clark*

Poster 373k: Investigation of Correlation Between Membrane Characteristics and Rejection Rate of Ions — ***Kiwoong Kim***

VAPOR PHASE SEPARATIONS - MATERIALS

Poster 373m: Petrified Hollow Fiber Membranes with Hierarchical Pores — ***Ching-En Ku***, *Lu Liu, Chen Zhang*

Poster 373n: Improving Propylene/Propane Separation Performances of Polycrystalline ZIF-8 Membranes Via Additive-Assisted Microstructural Modification — ***Donga Kang***, *Hae-Kwon Jeong*

Poster 373o: Dehydrated Channel Protein-Based Biomimetic Membranes with High Breathability and Protective Capability — ***Hyeonji Oh***, *Yu-Ming Tu, Benny D. Freeman, Manish Kumar*

Poster 373p: Effect of Grafting Density and Sidechain Length on Mechanical and Gas Transport Properties of Poly(ladder) Romps — ***Sherrie Qian***, *Kayla Storme, Sharon Lin, Francesco Maria Benedetti, Timothy Swager, Zachary Smith*

Poster 373q: Unexpectedly High Propylene-Selective Mixed-Matrix Membranes with Facile *in-Situ* ZIF-8 Filler Formation Process — ***Yinying Hua***, *Sunghwan Park, Hae-Kwon Jeong*

Poster 373r: Carbon Molecular Sieve Gas Separation Membranes Pyrolyzed from Aromatic Barrier Polymers — ***Gaurav Iyer***, *Chen Zhang*

Poster 373s: Separation of HFC-32, HFC-125, HFC-134a, HCFC-22, and HFO-1234yf Using Copolymers of Perfluoro(butenyl vinyl ether) and Perfluoro(2,2-dimethyl-1,3-dioxole) — ***Abby Harders***, *Erin Sturd, Luke Wallisch, Mark Shiflett*

Poster 373t: Iptycene-Based Polybenzimidazole Membranes for H_2/CO_2 Separation — ***Mengdi Liu***, *Ruilan Guo*

Poster 373w: Application of 2^6-Factorial Design Optimization for PVA Based Membrane Synthesis for CO_2/N_2 and CO_2/CH_4 Separation — *Iris Samputu, Bhavya Bhat,* ***F Handan Tezel***

Poster 373x: Feasibility Study of Membrane Reactor for Reverse Water Gas Shift By ZSM-5 Zeolite Membrane — ***Motomu Sakai***, *Masahiko Matsukata, Kyoka Tanaka*

VAPOR PHASE SEPARATIONS - PROCESSES

Poster 373y: Integrated Module Array with Facilitated Transport Membranes for Enhanced H_2 Recovery from Syngas — ***Yang Han***, *Yutong Yang, Ruizhi Pang, W.S. Winston Ho*

Poster 373z: Process Design and Optimization of Membrane-Cryogenic CO_2 Capture Process for Industrial CO_2 Emissions — ***Mun-Gi Jang***, *Jin-Kuk KIM*

Poster 373aa: Elucidating Key Factors Dominating Natural Gas Sweetening Efficiency of Membranes — ***Yang Liu***

Poster 373ab: Dynamic Modeling and Simulation of a Membrane Contactor for CO_2 Absorption — ***Wanderson Passos***, *Arioston Araújo de Morais Jr*

Poster 373ac: Respirator Cartridge Performance Testing for Chemicals of Potential Concern (COPC) at Higher Chemical Vapor Concentrations — ***Satish Nune***, *Michael Minette, Stephen Davidson, Angela Melville, Thomas Brouns, Eugene Morrey, Michael Zabel, Parker Jones, Zachary Way*

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(374) Poster Session: Separations Division

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, North Hall E

Ranil Wickramasinghe, Chair

Sponsored by: Separations Division

Poster 374b: Optimal MEA/Dipa /Water Blending Ratio for Minimizing Regeneration Energy in Absorption-Based Carbon Capture Process: Experimental Solubility and Thermodynamic Modeling — ***Mun Jihun***, *BeomJu Shin, Jong-Ho Moon, Kyung-Min Kim*

Poster 374c: Synthesis and Characterization of CO_2-Selective Membranes with Poly(ethylene formamidine) — ***Jingying Hu***, *Yang Han, Winston Ho*

Poster 374d: Responsive Membranes for Enhanced Capture and Detoxification of Water and Air Pollutants — ***Rollie Mills***, *J. Todd Hastings, Lindell Ormsbee, Thomas Dziubla, Dibakar Bhattacharyya*

Poster 374e: Optimal MEA/Dipa /Water Blending Ratio for Minimizing Regeneration Energy in Absorption Based Carbon Capture Process: Experimental Solubility and Thermodynamic Modeling — ***Mun Jihun***, *BeomJu Shin, Kyung-Min Kim, Jong-Ho Moon*

Poster 374f: Precise Control of Pore Size of Clinoptilolite and Separation of N2 from CH4 — ***Hiroshi Okaniwa***, *Yuki Jonoo, Yuki Oba, Satoshi Yoshida*

Poster 374g: Performance Analysis of a Multi-Bed PSA Process Using Silica-Based Adsorbents for CO_2 Capture from Off-Gas in Iron and Steel Industry — *Hongjoo Do, Jiwon Jung,* ***Jun-Ho Kang***, *Moonkyung Cho*

Poster 374h: Electrospun Polymer Fibers for Carbon Capture of CO_2 — ***Edward Huang***, *Jennifer Weiser, Amanda Simson*

Poster 374i: Carbon Capture from Residual Emissions Enabled By Facilitated Transport Membranes — ***Yang Han***, *W.S. Winston Ho*

Poster 374j: Application of Calcium Oxide-Based Bifunctional Catalytic Sorbent to Hydrogen Production — ***Pilseok Kim***, *Ki Bong Lee*

Poster 374k: Ca-Al Hydrotalcite-Based Mixed-Metal-Oxide for High-Temperature Carbon Dioxide Adsorption — ***Kuei Tan Lee***, *Ki Bong Lee*

Poster 374l: Selective Removal of Cs^+ in Acidic Nuclear Water Waste Using Epoxy Resins — ***Erwin Escobar***, *John Edward Sio, Rey Eliseo Torrejos, Khino Parohinog, Hern Kim, Wook-Jin Chung, Grace Nisola*

Poster 374m: Tunable H_2s/CO_2 Separation Using Sterically Hindered Amine Membranes — ***Shraavya Rao***, *Xuepeng Deng, Yang Han, Li-Chiang Lin, W.S. Winston Ho*

Poster 374n: Separation of Refrigerant R-410A Using Porous Materials: Thermodynamic Modeling and Breakthrough Experiments — ***Andrew Yancey***, *David R. Corbin, Mark Shiflett*

Poster 374o: Evaluating Transport Factors to Understand Electrochemical Nutrient Removal and Recovery from Synthetic Animal Wastewater — ***Sana Heydarian***, *Francesca Carney, Damilola Daramola*

Poster 374p: Intensified Water Purification Via Closed Loop Carbon Dioxide-Mediated Diffusiophoresis — ***Esai Lopez***, *Patryck Michalik, Shicheng Lyu, Alex D. Paulsen, Elizabeth Stewart, Andrew R Teixeira*

Poster 374q: Effect of Co-Ions on O_2 Gas Transport Properties of Cross-Linked Poly(ethylene oxide) — ***Taliehsadat Alebrahim***, *Narjes Esmaeili, Thien Tran, Haiqing Lin*

Poster 374r: Synthesis and Characterization of Multi-Ionic Block Copolymers for Chemical and Biological Protective Clothing Applications — *Karen Barrios Tarazona,* ***Gilberto Ramos Rivera***, *David Suleiman*

Poster 374s: Separation of Refrigerant Mixtures Using Extractive Distillation with Ionic Liquid Entrainers — *Ethan A. Finberg,* ***Mark B. Shiflett***

Poster 374u: Energy Efficient Advanced Separation Process of Solvent Mixture (Xylene, Butyl Acetate and Methyl Ethyl Ketone) Recovery/Re-Processing for Paint Industry — ***Abdur Rehman***

Poster 374v: CFD-PBM Simulation of Nickel-Manganese-Cobalt Hydroxide CO-Precipitation in CSTR — *Mohsen Shiea, Andrea Querio, Antonio Buffo, Gianluca Boccardo,* ***Daniele Marchisio***

Poster 374x: Energy-Efficient Process of Advanced Separation Technologies of Solvent Mixture (Xylene, Butyl Acetate and Methyl Ethyl Ketone) Recovery/Re-Processing for Paint Industry — ***Muhammad Haider***

(375) General Poster Session in Sensors

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, North Hall E

Ariel Furst, Chair
Jeffrey Halpern, Co-Chair

Sponsored by: Sensors for Sustainability

Poster 375a: Pd-Nanoparticle Enabled Optical Fiber Hydrogen Sensor for Subsurface Storage Conditions — ***Daejin Kim***, *Nathan Diemler, Ruishu Wright, Michael Buric, Paul Ohodnicki*

Poster 375b: Reshaping Molecularly Imprinted Polymers for Robust Sensing Performance — ***Cameron Malloy***, *Suchol Savagatrup, Ramon Castrejon Miranda*

Poster 375c: Dynamic Complex Emulsion Based Multiplexed Sensing Array for Environmental Contaminants Detection — ***Baishali Barua***, *Tyler Durkin, Suchol Savagatrup*

Poster 375d: Stress Sensor Synthesis Using Electropolymerized Molecularly Imprinted Polymers — ***Grace Dykstra***, *Yixin Liu*

Poster 375e: Enzymatic Electrochemical Sensing for Fish Freshness Using Macro-Porous NiO Electrodes — ***Anuja Tripathi***, *Anastasia L. Elias, Abebaw B. Jemere, Kenneth D. Harris*

Poster 375f: Construction of a Sensor for Rapid and Online Measurement of Dissolved Methane in Bioreactor Systems — ***Robert Bertrand***, *Lisa Stephanie Dizon, Rafael Hernandez, Mark Zappi, Emmanuel Revellame*

(376) Andrew Chase Award II (Invited Talks)

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-228A

Xuejun Pan, Chair

Sponsored by: Forest and Plant Bioproducts Division

3:30 Paper 376a: Exploiting Synergies of Anionic and Cationic Biomaterials for Oxygen and Water Vapor Barrier Properties — ***J Carson Meredith***

4:00 Paper 376b: Improvements in Oil and Grease Resistance (OGR) Test Methodology for Waterborne Barrier Coatings — ***Allyson Marianelli***

4:30 Paper 376c: Value-added Biochemicals and Functional Biomaterials from Biowaste — ***Zhaohui Tong***

5:00 Paper 376d: Conversion of Lignocellulosic Biomass to Value-Added Chemicals and Materials in Inorganic Ionic Liquid (molten salt hydrate) — ***Xuejun Pan***

(377) Catalyst Design, Synthesis, and Characterization VI: Structure/activity relationships II

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-127C

Jean-Sabin McEwen, Chair
Weijian Diao, Co-Chair
Nathaniel Eagan, Co-Chair

Sponsored by: Catalysis

3:30 Paper 377a: Light Olefin Oligomerization Via Isolated Ni^{2+} Sites on Well-Defined Lacunary Defects of Wells Dawson Polyoxometalate — ***Yoonrae Cho***, *Galiya Magazova, Jessica A. Muhlenkamp, Allen Oliver, Jason Hicks*

3:48: Break

4:06 Paper 377c: Selective Hydrogenation of Cinnamaldehyde over a Bimetallic Single Atom Catalyst Synthesized Via Chelate Fixation Participants — ***Brian Vakili***, *Shima Oruji, Abolfazl Shakouri, John Regalbuto, Dr. Christopher T. Williams*

4:24 Paper 292h: Oxygen and Sulfur Reduction Activities of High N-Content Nanoporous Fe,N-Carbon Electrocatalysts Correlate with Atomic-Scale Compositions and Structures — ***Bradley F. Chmelka***, *Shona Becwar*

4:42 Paper 377e: Novel Synthesis of Catalytic Active Sites in Flow for on-Demand Hydrogen Production from Ammonia. — ***Joseph El-Kadi, Laura Torrente-Murciano***

5:00 Paper 377f: Characterizing Rh Single-Atom Catalysts on γ-Al_2O_3 Using Density Functional Theory and CO Probe Molecule IR Spectroscopy — ***Alexander Hoffman***, *Chithra Asokan, Nicholas Gadinas, Emily Schroeder, Steven V. Nystrom Jr., Andrew (Bean) Getsoian, Phillip Christopher, David Hibbitts*

5:18 Paper 377g: Rational Intermetallic Compounds Design for Selective Hydrogenation of Cinnamaldehyde — ***Sijie Guo***, *Siris Laursen*

5:36 Paper 377h: Method for Precise Tuning of Shell Thickness on Silica-Encapsulated Gold Core-Shell Nanoparticles and Impact on Catalytic Performance — ***Ellis Hammond-Pereira***, *Steven Saunders*

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(378) Fundamentals of Catalysis and Surface Science VI: Oxides and metal-support interactions

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-128B

Joseph Gauthier, Chair
Ana Colaco Morais, Co-Chair

Sponsored by: Catalysis

3:30 Paper 378a: Generalized Design Principles for Designing Metal/Support Interfaces with Active Site Specificity — ***Asmee Prabhu***, *Kah Meng Yam, Lavie Rekhi, Luan Q. Le, Quang Thang Trinh, Tej Choksi*

3:50 Paper 378b: Ni Adsorption, Ingress, and Egress on $SrTiO_3$ Single Crystals — ***Bader Alayyoub***, *Tianyu Cao, Ohhun Kwon, John Vohs, Raymond J. Gorte, Aleksandra Vojvodic*

4:10 Paper 378d: Exploring the Oxygen Surface Reactivity on Non-Octahedral Sites in Transition Metal-Oxides — ***Neha Bothra***, *Kirsten Winther, Michal Bajdich*

4:30 Paper 378e: Hydrogen Spillover and Its Relation to Hydrogenation Catalysis — ***Max Huelsey***, *Ning Yan*

4:50 Paper 378f: Mechanistic Details of the Selective Deoxygenation of Pentanoic Acid Using Molybdenum Oxide as a Catalyst: The Complex Role of the Local Hydrogen Concentration — ***Laura A. Gomez***, *Caleb Q. Bavlnka, Ethan Zhang, Bin Wang, Steven Crossley*

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(379) Green Chemical Reaction Engineering for Sustainability

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-128A

Peter Valdez, Chair
Wan-Ting Chen, Co-Chair
Hsu Chiang, Co-Chair

Sponsored by: Reaction Engineering

3:30 Paper 379a: Kinetic Modeling in Mixing Feedstocks of Hydrothermal Liquefaction — *Seshasayee Mahadevan Subramanya,* ***Peter Guirguis***, *Phillip E. Savage*

3:50 Paper 379b: In Situ Product-Removal for the Enzymatic Biodegradation of Poly(ethylene terephthalate) (PET) Via a Membrane Reactor — ***Christian Ayafor***, *Allen Chang, Akanksha Patel, Dongming Xie, Margaret J. Sobkowicz, Hsi-Wu Wong*

4:10 Paper 379c: Oxidative Functionalization of Long-Chain Alkanes By Pulsed Plasma Discharges at Atmospheric Pressure — ***Darien Nguyen***, *Panagiotis Dimitrakellis, Mary Watson, Michael Talley, Dionisios Vlachos*

4:30 Paper 379d: Green Selective Oxidation Using Heterogenous Catalytic Sonochemistry — *Umesh Jonnalagadda, Qianwenhao Fan, Xiaoqian Su,* ***James Kwan***, *Paul Liu*

4:50 Paper 379e: Material Recycling of Polycarbonate from Electronic Waste Using Density Separation and Safer Solvents — *Evan Yu,* ***Wan-Ting Chen***

5:10 Paper 379f: Outperformance of a Microwave-Heated Reactor over a Conventional Reactor in Steam and Sorption Enhanced Reforming of Ethanol over Ni-Silica-Aerogel Catalysts. — *Merve Sariyer, Naime Aslı Sezgi,* ***Timur Dogu***

5:30 Paper 379g: Simulation and Optimization of Volatile Fatty Acid Upgrading Strategies for Sustainable Transportation Fuel Production — ***Jacob Miller***, *Stephen Tifft, Matthew Wiatrowski, Pahola Thathiana Benavides, Nabila Huq, Earl Christensen, Teresa Alleman, Cameron Hays, Jon Luecke, Violeta Sànchez i Nogué, Eric Karp, Troy Hawkins, Avantika Singh, Derek Vardon*

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(380) In Honor of the 2021 CRE Practice Award Winner (Invited Talks)

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-127A

Klavs Jensen, Chair
Michael Harold, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

3:30 Paper 380a: Reaction Kinetics for Fluidized Bed Reactor Scale-up — ***Daniel Hickman***, *Paul Witt*

3:55 Paper 380b: Heterogeneous Catalysis for Pharmaceutical Scale Flow Processes — ***Joel Hawkins***

4:20 Paper 380c: Development of a Platform for Aerobic Processes — ***Joeseph Martinelli***

4:45 Paper 380d: Process Development and Scale-up of a Photochemical Reaction for Drug Substance Manufacturing — ***Jonathan P. McMullen***

5:10 Paper 380e: Optimization of Continuous Organic Synthesis By Integrating Automation, Machine Learning, and Robotics. — ***Klavs Jensen***

5:35 Paper 380f: Design and Selection of Continuous Reactors for Pharmaceutical Manufacturing — ***Martin Johnson***

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(381) In Honor of the 2022 CRE Early Career Investigator Award winner (Invited Talks)

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-127B

Randall Meyer, Chair
Stuart L. Soled, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

3:30 Paper 381a: Chemistry and Process Learnings for Molecular Weight Growth Using Solid Acid Catalysts — ***Matthew S. Mettler***

3:50 Paper 381b: Evaluating Bipolar Membrane Electrolyzers for Seawater Electrolysis and Undersea O_2 Production — ***Adam Nielander***, *Daniela Marin, Joseph Perryman, Michaela Burke Stevens, Thomas Jaramillo*

4:10 Paper 381c: Nickel-Catalyzed Oligomerization of Di- and Trisubstituted Olefins — ***Suzzy Ho***

4:30 Paper 381d: Reaction-Diffusion-Deactivation within Hierarchical Zeotypes for Bulky Hydrocarbon and Oxygenate Upgrading — *Hayat Adawi,* ***Michele Sarazen***

4:50 Paper 381e: Structure-Property Relationships That Influence Platinum Cluster Stability in All-Silica or Highly Siliceous Zeolites — ***Allen Burton***

5:10 Paper 381f: CO_2 Conversion in Pressure-Tunable Organic CO_2-Expanded Electrolytes — ***James Blakemore***, *Kevin C. Leonard, Bala Subramaniam*

5:30 Paper 381g: Experimentally Simulating Dehydrogenation Catalysis in H_2-Removal Membrane Reactors, without Using Membrane Reactors — ***Aaron Sattler***

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(382) Multiphase & Liquid Phase Reaction Engineering

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-223

Joris Thybaut, Chair
Simon Kuhn, Co-Chair

Sponsored by: Reaction Engineering

3:30 Paper 382a: Slug-Flow Manufacturing of Uniform Nickel-Cobalt-Manganese Precursor Microcrystals for Battery Cathodes — *Mingyao Mou, Arjun Patel, Selma Saleh, Jethrine Mugumya, Sourav Mallick, Michael L. Rasche, M. Parans Paranthaman, Herman Lopez, Ram Gupta,* ***Mo Jiang***

3:50 Paper 382b: Investigate the Solid Phase Distribution and Turbulent Parameters in Slurry Bubble Column with/without Dense Internals Using Radioactive Particle Tracking (RPT) Technique — *Omar Farid, Muthanna Al-Dahhan, Alexandre Velo, Binbin Qi,* ***Sebastian Uribe***

4:10 Paper 382c: Impact of Variable Gas Mixtures on Bubble Size Distribution and Mass Transfer in Gas Fermentation Reactors — ***Hari Sitaraman****, Malik Hassanaly, John Parra-Alvarez, Mohammad J. Rahimi, Jonathan Stickel*

4:30 Paper 382d: Turbulent Reactive Transport Effects in Crystallization Processes — ***Benaiah Anabaraonye****, Jakob Roar Bentzon, Jens H Walther, Simon Ivar Andersen*

4:50 Paper 382e: Continuous Emulsification in 3DP Fixed Beds: Drop Size Distribution and Emulsification Efficiency — ***Kaitlin Kay****, Andres Hyer, Robert McMillin III, James K. Ferri*

5:10 Paper 382f: A Chemical Kinetic Mechanism for Ethanol Oxidation in Supercritical Water — ***Andrew Mansfield***

5:30 Paper 382g: Simulating the Ultrasound Assisted Depolymerization of Biomass Using Reduced Order Multiscale Models. — ***Tej Choksi****, Ari Fischer, Prince N. Amaniampong, Sabine Valange, Roberto Batista da Silva Jr.*

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(383) Honorary sessions for Keith Gubbins' 85th birthday (Invited Only)

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-222B

Kaihang Shi, Chair
Liangliang Huang, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

3:30 Paper 383a: Computational Design of Peptides As Biomarkers, Sensors, Detectors and Drugs — ***Carol Hall***

3:50: Break

4:10 Paper 383c: Capillary Condensation and Hysteresis in Nanoporous Materials: New Simulations and New Insights — *Zhao Li,* ***Randall Snurr***

4:30 Paper 383d: Robust Phase Equilibria in Reactive Non-Ionic and Ionic Systems Relevant to Pharmaceutical Applications — ***Amparo Galindo***

4:50 Paper 383e: Charting the Design Space of Chemically-Heterogeneous Surfaces That Manipulate Water-Mediated Interactions — ***M. Scott Shell***

5:10 Paper 383f: Wetting and Electrowetting of Polyelectrolyte Complex Coacervates on Solid Surfaces — *Christopher Balzer, Pengfei Zhang,* ***Zhen-Gang Wang***

5:30 Paper 383g: Free Energy Barriers for Anti-Freeze Protein Engulfment: A Model for the Effects of Supercooling, Footprint Size, and Neighbor Distances — *Hossam Farag,* ***Baron Peters***

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(384) Chemical Engineering Laboratory Experiments and Instruction

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, W-105B

Tracy Carter, Chair
Beth Rundlett, Co-Chair
Stephanie Loveland, Co-Chair

Sponsored by: Undergraduate Education

3:30: Welcoming Remarks

3:32 Paper 384a: A State-of-the-Art Pilot-Scale Distillation Column for the Unit Operations Laboratory at the University of Kansas — ***Felipe Anaya****, David M. Griffin, Mark B. Shiflett*

3:50 Paper 384b: Design Your Own Experiment: An Alternative Experiment for Seniors in Process Engineering Laboratory — ***Alex Bertuccio***

4:08 Paper 384c: Design Projects in the Unit Operations Laboratory — ***Stephanie Loveland****, Kristin Stoner*

4:26 Paper 384d: Enhance Safety Knowledge and Mindset through the ChE Undergraduate Laboratory Courses — ***Chijuan Hu***

4:44 Paper 384e: Continued Improvement of the Chemical Engineering Undergraduate Laboratories at the University of Texas at Austin — ***Carlos Landaverde-Alvarado***

5:02 Paper 384f: A Novel Approach for Laboratory Experiments in Process Dynamics and Control — ***Felipe Anaya****, David M. Griffin, Mark B. Shiflett*

5:20 Paper 384g: Green Cubesat Propulsion: Using Hands-on Experimentation to Develop Knowledge and Interest in STEM and NASA Career Opportunities. — ***Greg Ogden***

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(385) Best Practices for LGBTQ+ & Ally Resource Groups

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-231B

Alon McCormick, Chair

Sponsored by: LGBTQ+ and Allies Community

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(386) WIC Drop-in Mentoring

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-232C

Caroline Szczepanski, Chair

Sponsored by: Women in Chemical Engineering Committee (WIC)

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(387) Biomolecules at Interfaces II

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-125B

Julie N. Renner, Chair
Roberto Andresen Eguiluz, Co-Chair
Bernardo Yanez Soto, Co-Chair

Sponsored by: Interfacial Phenomena

3:30 Paper 387a: Lung Surfactant Interfacial Properties and Morphology: The Effects of Inflammation Derived Contaminants — ***Steven Iasella****, Clara Ciutara, Sourav Barman, Joseph Zasadzinski*

3:45 Paper 387b: Rheology of Layered Biological Lipids/Surfactants Using Quartz-Crystal Microbalance with Dissipation — *Silvia Jonguitud-Flores, Rodrigo Velez-Cordero, Gabriel Espinosa-Perez, Clayton Radke,* ***Bernardo Yanez Soto***

4:00 Paper 387c: Inactivation of Lung Surfactant By Phospholipase-Catalyzed Degradation — ***Julia Fisher****, Todd Squires*

4:15 Paper 387d: Stability of Mab-Surfactant at the Air-Water Interface Under Competitive Adsorption and Controlled Flow Deformations — *Ying-Heng Tein,* ***Norman J. Wagner***

4:30 Paper 387e: Probing Adsorption of Monoclonal Antibodiesat Water-Oil Interfaces Via Dynamic Surface Tensiometry and Spatially Resolved NMR Spectroscopy — *Jamini Bhagu, Samuel Grant,* ***Hadi Mohammadigoushki***

4:45 Paper 387f: Nanomechanics of Macromolecular Assembly of Synovial Fluid Components on Articular Cartilage Extracellular Matrix — ***Syeda Tajin Ahmed****, Roberto Andresen Eguiluz*

5:00 Paper 387g: Investigating Bio-Nano Interactions of Pegylated Cationic Polyamidoamine (PAMAM) Dendrimers within Articular Cartilage — ***Simone Douglas-Green****, Juan A. Aleman, Brandon M. Johnston, Alan Grodzinsky, Paula T. Hammond*

5:15 Paper 387h: Competitive adsorption between monoclonal antibodies and non-ionic surfactants at the air-water interface — ***Benjamin Thompson****, Tingting Wang, Ken K. Qian, Yun Liu, Norman J. Wagner*

5:30 Paper 387i: Evaluating the Combined Impact of Temperature and Application of Interfacial Dilatational Stresses on Surface-Mediated Protein Particle Formation in MAb Formulations — ***Valerie Griffin****, Kimberly Merritt, M. Coleman Vaclaw, Neal Whitaker, David Volkin, Maria Olu Ogunyankin, Samantha E. Pace, Prajnaparamita Dhar*

5:45 Paper 387j: Elastic Response of Synovial Fluid Nanofilms on Model Oxide Surfaces Is Compromised When Cleaving Glycoproteins and Glycosaminoglycans — *Amar Mann, Ariell Smith, Joyce Saltzherr, Arvind Gopinath,* ***Roberto Andresen Eguiluz***

(388) Data Science in Complex Fluids and Complex Flows

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-232A

Safa Jamali, Co-Chair
Lilian Hsiao, Co-Chair

Sponsored by: Fluid Mechanics

3:30 Paper 388a: Data-Driven Modeling of a Dynamic System with Extreme Events through Neural Networks in an Atlas of Charts — ***Andrew Fox****, Michael Graham*

3:50 Paper 388b: Stabilized Neural ODEs for Data-Driven Reduced-Order Modeling of Plane Couette Flow — ***Alec Linot****, Michael Graham*

4:10 Paper 388c: Automated High-Throughput Microrheology for Material Formulation — *Yimin Luo, Alexandra V. Bayles, Mengyang Gu, Yue He, Rhett L. Martineau, Maneesh K. Gupta, Todd Squires, Megan T. Valentine,* ***Matthew Helgeson***

4:30 Paper 388d: Rigid Structures in Frictional Dense Suspensions — ***Abhinendra Singh****, Michael van der Naald, Juan J. de Pablo, Heinrich M. Jaeger*

4:50 Paper 388e: Using Co-Optimized Machine Learned Manifolds for Modeling Chemically Reacting Flows — ***Bruce Perry****, Marc Henry de Frahan, Shashank Yellapantula*

5:10 Paper 388f: A Deep Learning Framework for Predicting Fluid Flow in Porous Membranes — ***Serveh Kamrava****, Muhammad Sahimi, Pejman Tahmasebi*

5:30 Paper 388g: Bayesian Optimisation for Plug Performance of Coiled Tubes at Low-Reynolds-Number — ***Nausheen Basha****, Tom Savage, Miguel Ángel de Carvalho Servia, Jonathan McDonough, Ehecatl Antonio del Rio Chanona, Omar K. Matar*

(389) Electrochemical Fundamentals: Faculty Candidate Session II

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-232B

Wenzhen Li, Chair
Shuya Wei, Co-Chair

Sponsored by: Electrochemical Fundamentals

3:30 Paper 389a: In Situ Characterization of Interfacial Properties in (Photo)Electrochemical Systems — ***Elizabeth Corson***

3:45 Paper 389b: Elucidating Structure-Property Relationships in Photoelectrochemical Energy Conversion Systems — ***Aisulu Aitbekova****, Harry A. Atwater*

4:00: Intermission

4:15 Paper 389d: Defect-Rich Ultrathin Nicofe Nanosheets for Efficient Oxygen Evolution Catalysts — ***Lemma Tufa****,* ***Jaebeom Lee***

4:30 Paper 389e: Understanding Electrochemistry from the Atomic to Macroscopic Scale — ***Joakim Halldin Stenlid, PhD***

4:45: Break

5:00 Paper 389i: Designing M-N-C Electrocatalysts with Inspiration from Thermal and Molecular Catalysis — ***Jason Bates***

5:15 Paper 389f: Activity, Selectivity, and Stability: Tracing New Routes for Electrocatalysts Design By Using First-Principles Methods — ***Roberto Schimmenti***

5:30 Paper 389g: Combining Physics Driven and Graph Theory-Based Methodologies for Modeling Complex Heterogeneous Electro-Catalytic Surfaces — ***Siddharth Deshpande***

5:45 Paper 389h: Role of Water Molecules in Enabling Vehicular Transport Mechanism in Polynorbornene-Based Anion Exchange Membrane — ***Zhongyang Wang***

(390) Microscale Transport Processes

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-230

Dmitry I. Kopelevich, Chair
Aashish Priye, Co-Chair

Sponsored by: Transport Processes

3:30 Paper 390a: Statistical Inference of Transport Mechanisms from Time Series of Solute Trajectories in Polymer Membranes — *Benjamin J. Coscia, Nathanael Schwindt,* ***Michael R. Shirts***

3:48 Paper 390b: Lose-Lose Diffusion in Complex Networks — ***Tobias Dwyer****, Timothy C. Moore, Sharon C. Glotzer*

4:06 Paper 390c: Connection between Local Dynamic Environments & Relaxation Mechanism — ***Kelly Badilla****, Andreas Bommarius, Marcus T Cicerone*

4:24 Paper 390d: The Impact of Configurational Entropy on Point Defect Thermodynamics and Diffusion in Crystalline Silicon — *Jinping Luo, Lijun Liu,* ***Talid Sinno***

4:42 Paper 390e: Model for Nanoparticle Aggregation in Confined Geometries — ***Vi Nguyen****, Ngoc Hong Pham, Dimitrios Papavassiliou*

5:00: Break

5:18 Paper 390g: Assembly of Protocell-like Vesicles in Microscale Hydrothermal Pores Via Synergistic Trapping and Chaotic-Mixing — ***Vijay Ravisankar****, Yassin Hassan, Victor Ugaz*

5:36 Paper 390h: Effect of Minerals on Static Adsorption of a Novel Gemini Surfactant — ***Shams Kalam****, Sidqi Abu-Khamsin, Muhammad Shahzad Kamal, Shirish Patil, Syed Hussain, Emad W. Al Shalabi*

(391) Particulate and Multiphase Flows: Colloids and Polymers

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-231C

Ryan Poling Skutvik, Co-Chair
Michelle Calabrese, Co-Chair

Sponsored by: Fluid Mechanics

3:30 Paper 391a: Defining the Structure, Rheology and Properties of Colloidal Rod Systems during Dynamic Phase Transitions — *Shiqin He, Marco Caggioni, Seth Lindberg,* ***Kelly M. Schultz***

3:50 Paper 391b: A Thermodynamically Consistent, Microscopically-Based Model of Aggregating Particle Suspension Rheology — ***Soham Jariwala****, Norman J. Wagner, Antony N. Beris*

4:10 Paper 391c: Electrochemical Jamming in Dense Suspensions: Training and Memory — ***Hojin Kim****, Hongyi Zhang, Garrett Grocke, Shrayesh Patel, Heinrich M. Jaeger, Stuart J. Rowan*

4:30 Paper 391d: The Role of Brittility in the Yielding of Polymeric, Colloidal, and Composite Materials — *Krutarth Kamani,* ***Simon Rogers***

4:50 Paper 391e: Stress Relaxation and Yielding Behavior of Gelatin Nanoparticles/2D Clay Hybrid Colloidal Gels — ***Gelareh Rezvan****, Mohsen Esmaeili, Monirosadat Sadati, Nader Taheri-Qazvini*

5:10 Paper 391f: Elastic Turbulence in Structurally-Complex Porous Media: Linking Pore-Scale Flow Behavior to Macroscopic Flow Resistance — *Christopher Browne, Emily Chen,* ***Sujit Datta***

5:30 Paper 391g: Understanding High Shear Impact to Sodium Hyaluronate Size Control and Formulations — ***Mohannad Kadhum****, Jack Kochevar, Kamlesh Patel, Ryan Swanson, Steve Laninga*

(392) Remediation of Emerging Contaminants and Legacy Compounds II

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-225B

Alexander Dowling, Chair
Sage Hiibel, Co-Chair
Robert Peters, Co-Chair

Sponsored by: Water

3:30 Paper 392a: Lab- and Pilot-Scale Sulfate-Reducing Bioreactors Treating Acid Mine Drainage from an Abandoned Nevada Gold Mine — ***Thomas Kaps, Sage Hiibel***

3:55 Paper 392b: Weathering Induced Changes in Microplastic Dispersity and Pollutant Uptake Capacity — *Philip J. Brahana, Ahmed Al Harraq,* ***Bhuvnesh Bharti***

4:20 Paper 392c: Critical Review of the Fenton Oxidation Process for Industrial Wastewater Treatment — ***Amany M. Naguib,*** *Soha A. Abdel-Gawad,* ***Mohamed Mostafa, Ahmed Mahmoud, Robert Peters***

4:45 Paper 392d: Removal of Arsenic and NORM from Water with Novel Clay Adsorbents Developed Using Camd — ***Ubadire Onyemaobi,*** *Urmila Diwekar, Rajib Mukherjee, Narendra Boppana*

5:10 Paper 392e: Understanding the Mechanism of Adsorptive Selectivity of Arsenic over Phosphorous Oxoanions By Fe(III)-Crosslinked Chitosan Using DFT — ***Obinna Nwokonkwo,*** *Christopher Muhich*

(393) Sustainability Fundamentals and Metrics Applications

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-225A

Yinlun Huang, Chair
Mariano Martin, Co-Chair
Heriberto Cabezas, Co-Chair
Fernando V. Lima, Co-Chair

Sponsored by: Fundamentals

3:30 Paper 393a: Integrated Sustainability Assessment: Exergy, Emergy, Life Cycle Assessment — ***Natalia Cano,*** *Camilo A. Franco, Farid B Cortés, Krisztián Baracza, Jo Dewulf, Heriberto Cabezas*

3:55 Paper 393b: Interaction Analysis in Multiscale Sustainability Assessment — ***Mahboubeh Moghadasi,*** *Yinlun Huang*

4:20 Paper 393c: Optimization Based Selection of Industrial Biosolids Treatment and Valorization Pathways to Meet International Discharge Standards for Heavy Metals — ***Nivinya Hemachandra,*** *Dhabia Al-Mohannadi, Debalina Sengupta*

4:45 Paper 393d: Modeling and Analysis of Anaerobic Membrane Bioreactor (AnMBR) for Integrated Resource Recovery from Wastewater — ***Madison E. Kratzer,*** *Prathap Parameswaran, Vikas Khanna*

5:10 Paper 393e: A Closed Loop Case Study of Food Waste Management in Singapore — ***Yen Wah Tong,*** *Hailin Tian*

(394) Division Plenary: Food, Pharmaceutical, and Bioengineering Division (Invited Talks)

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-129AB

Ian Wheeldon, Chair
Wilfred Chen, Co-Chair
Brad Bundy, Co-Chair
Mark Brynildsen, Co-Chair

Sponsored by: Food, Pharmaceutical & Bioengineering Division

3:30 Paper 394a: Division Plenary: Synthetic Biology: Putting Synthesis into Biology — ***Huimin Zhao***

4:20 Paper 394b: Early Career Award: Discovery, Domestication, and Engineering of Diverse Microbes for a Circular Economy — ***Mark Blenner***

4:45 Paper 394c: Area 15a Plenary: Opportunities for Cell Engineering for Cellular Agriculture — ***David L. Kaplan***

5:10 Paper 394d: Area 15c Plenary: Outsmarting pathogens with protein engineering: lessons from pertussis, cytomegalovirus and coronavirus. — ***Jennifer Maynard***

5:35 Paper 394e: Area 15d/e Plenary: Tissue-Inspired Synthetic Biomaterials — ***Shelly Peyton***

(395) Properties and Phase Equilibria for Fuels and Petrochemicals

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, W-102C

Wade Vincent Wilding, Chair
M R Riazi, Co-Chair

Sponsored by: Fuels and Petrochemicals Division

3:30 Paper 395a: Polyazeotropy for Binary Mixtures: Methanol and Diethylamine — ***Nooram Anjum,*** *Shigeo Oba, Toshihiko Hiaki, Chau-Chyun Chen*

3:48 Paper 395b: The Investigation of the Effects of Asphaltene Molecular Properties on Asphaltene-Solids Heterogeneous Interaction — ***Weiyi Kong,*** *Rizwanur Rahman, Michael P. Hoepfner*

4:06 Paper 395c: The Ideal Gas Contribution to Liquid Heat Capacity — ***Cassandra Guffey,*** *Joseph Bloxham, Neil Giles, Thomas Knotts IV, Wade Vincent Wilding*

4:24 Paper 395d: Modeling of Nitrogen + Fuel Phase Behavior Using the Helmholtz-Energy-Explicit Equation of State — ***Aaron J. Rowane,*** *Ian H. Bell*

4:42 Paper 395e: Improving the Capability of Process Simulators to Represent Solid-Fluid Equilibria Applied to Natural Gas Liquefaction: The Methane + Neopentane System at Low Temperature — *David Bluck,* ***Seiya Hirohama,*** *Nevin Gerek Ince, Marco Campestrini, Paolo Stringari, Freddy Garcia, Jean-Jacques Bartuel*

5:00 Paper 395f: Methane Mass Transfer in Liquid Hydrocarbon Mixtures – Measurement and Modeling in Synthetic Porous Media — ***Sheng Hu,*** *Theodore Tsotsis, Kristian Jessen*

5:18 Paper 395g: Exploring Liquid Crystalline Phase Behavior of Pyrene Pitch Oligomers Isolated Via Supercritical Extraction — ***Graham W. Tindall,*** *Jefferson T. Giles II, Adam S. Gross, Yunlong Zhang, Amy C. Clingenpeel, Kazem V. Edmond, Manesh Gopinadhan, Stuart E. Smith, David Perkins, Jonathan D. Saathoff, Mark C. Thies*

(396) Value-Added Chemicals from Natural Gas I

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, W-103A

Dushyant Shekhawat, Chair
Goetz Veser, Co-Chair
Jianli Hu, Co-Chair
Daniel Haynes, Co-Chair

Sponsored by: Fuels and Petrochemicals Division

3:30 Paper 396a: Towards Rational Design of Metal-Embedded Zeolite Catalyst for Improved Catalytic Performance in Microwave-Assisted Methane Dehydro-Aromatization — ***Sanjana Karpe,*** *Xinwei Bai, Brandon Robinson, Jianli Hu, Goetz Veser*

3:49 Paper 396b: Deactivation Study of Mo-HZSM-5 Catalyst for Microwave-Assisted Methane Aromatization: Effect of Reaction Parameters — ***Ashraf Abedin,*** *Pranjali Muley, Victor Abdelsayed, Xinwei Bai, Hari Paudel, Daniel Haynes*

4:08 Paper 396c: Ethane Dehydroaromatization with CO_2 Co-Feed over Microwave Synthesized Core-Shell Transition-Metal-Carbide@ZSM-5 Material — ***Ashley Caiola,*** *Brandon Robinson, Sean Brown, Jianli Hu*

4:27 Paper 396d: Enhanced Dry Reforming of Methane Using Pseudo Catalytic Metal Oxide and Nanoparticles — ***Pinak Mohapatra,*** *Qichang Meng, Anuj Joshi, Sonu Kumar, Patricia Loughney, Ashin Sunny, Lang Qin, Zhuo Cheng, Vicky Doan-Nguyen, Liang-Shih Fan*

4:46 Paper 396e: Low Temperature "Super-Equilibrium" Reforming of Methane through Chemical Looping — ***Luke Neal,*** *Chongyan Ruan, Fanxing Li*

5:05 Paper 396f: Microwave Catalytic Conversion of Acetylene for Co-Production of Hydrogen and Carbon Nanotubes — ***Sonit Balyan***, *Changle Jiang, Ashley Caiola, Jianli Hu*

5:24 Paper 396g: Enhanced Methane Decomposition over Transition Metal-Based Tri-Metallic Catalysts for the Production of Cox Free Hydrogen — ***Basem Al Alwan***, *Mumtaj Shah, Mohd Danish, Mohammed K. Al Almesfer, Mohammed Khan, Varagunapandiyan Natarajan*

5:43: Break

(397) Integrated Process Engineering and Economic Analysis

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-228B

Yizu Zhu, Chair
Jerry Kaczur, Co-Chair
Qi Zhang, Co-Chair

Sponsored by: Green Process and Product Engineering

3:30: Break

3:45 Paper 397b: Optimization of Nonlinear, Variable-Cost Network Models of the Chemical Manufacturing and Refining Industry — ***Alkiviadis Skouteris***, *Ioannis Giannikopoulos, David Allen, Michael Baldea, Mark Stadtherr*

4:00 Paper 397c: Techno-Economic Analysis and Life Cycle Assessment of Bio-Based Hydrogen Production from Integrated Dark-Fermentation and Microbial Electrolysis Cells — ***Xinyu Liu***, *Adarsh Bafana, Pingping Sun, Amgad Elgowainy, Katherine J. Chou, Alexander Beliaev, Eric Hill, Steven W. Singer, Eric Sundstrom*

4:15: Break

4:30 Paper 397e: A Simple Framework to Explore the Financial and Technical Challenges of Decarbonization & Sustainability — ***Carlos Villa***, *Narayan Ramesh*

4:45 Paper 397f: Evaluation and Optimization of Decarbonization Strategies in Indian Steel Industry for Sustainable Scenarios — ***Sydney Johnson***, *Lingyan Deng, Emre Gençer*

5:00 Paper 397g: Techno-Economic Feasibility Analysis of Liquid Metal-Based Methane Pyrolysis Process — ***Semie Kim***, *Young-Il Lim, Uen-Do Lee, Youn-Bae Kang, Sungwon Kim*

5:15 Paper 397h: Process Design and Economic Analysis for the Retrofitting of a Hydrogen Plant with CO_2 Capture — ***Joohwa Lee***, *Haryn Park, Seokwon Yun, Jin-Kuk KIM*

(398) AIChE Journal Futures: New Directions in Chemical Engineering Research (Invited Talks)

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-224AB

David Sholl, Chair

Sponsored by: Publication Committee

3:30 Paper 398a: Incorporation of Cellulose Nanocrystals and Reactive Surfactants for Improved Pressure Sensitive Adhesive Performance — ***Caroline Szczepanski***, *Justin Hamlin, Md Nuruddin, Volodymyr V. Tarabara*

3:49 Paper 398b: Engineering the Tumor Cell Niche to Study Dormancy in Metastatic Breast Cancer — ***Shreyas Rao***

4:08 Paper 398c: Accelerating the Development of High-Performing Dynamic Electrochemical Processes via Bayesian Optimization — ***Miguel Modestino***, *Daniel Frey*

4:27 Paper 398d: Mathematical Modeling of the Effects of Wnt-10b on Bone Metabolism — ***Ashlee Ford Versypt***, *Carley V. Cook, Mohammad Aminul Islam, Brenda J. Smith*

4:46 Paper 398e: Grid-Responsive Smart Manufacturing: A Perspective for an Interconnected Energy Future in the Industrial Sector — ***Blake Billings***, *Kody Powell*

5:05 Paper 398f: Science-Based Design of Experiments and Data Analytics for Molecular-to-Systems Engineering — ***Alexander Dowling***, *Jialu Wang, Xinhong Liu, William Phillip, Jonathan Ouimet, Laurianne Lair*

5:24 Paper 398g: AIChE Journal Futures: Placeholder 7

5:43 Paper 398h: AIChE Journal Futures: Placeholder 8

(399) Plenary Session: Turbulence and Mixing – In Memory of Professor Robert Brodkey II (Invited Talks)

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-222C

Stuart L. Cooper, Co-Chair
Jennifer Curtis, Co-Chair

Sponsored by: Miscellaneous

3:30: Introduction: Stuart Cooper, Ohio State University

3:35 Paper 399b: Cross-Gradient Transport and Mixing in Turbulent Shear Flows — ***James Hill***, *Rodney Fox, Michael G. Olsen*

3:55 Paper 399c: On Robert Brodkey, suspending solids and transporting slurries — ***Harry Van den Akker***

4:20 Paper 399d: Effects of Shear Flow Structure on Turbulent Transport and Mixing — ***Dimitrios Papavassiliou***, *Oanh Pham, Quoc T. Nguyen*

4:45 Paper 399e: Turbulence and Mixing - Honoring Professor Robert Stanley Brodkey — ***Charles Petty***

5:10 Paper 399f: Laminar Chaotic Mixing in 3D Systems - A Thirty-Year Conversation with Robert Brodkey — ***Fernando Muzzio***

5:35 Paper 399g: Fundamental Studies of Laminar Stagnation Flows and Design of Stagnation-Flow Reactors — ***Triantafillos Mountziaris***

6:00: Conclusion: Jennifer Curtis, University of California-Davis

(400) AIChE Management Award Recipient Presentation Session: Nuclear Energy in a Sustainable World

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-229AB

Joseph Cramer, Chair
Mark Swientoniewski, Co-Chair
George Newcomb, Co-Chair

Sponsored by: Management Division

3:30 Paper 400a: Award Presentation and Brief Introductory Remarks — ***Mark Swientoniewski***

3:45 Paper 400b: Life & Legacy of a Transformative Nuclear Career — ***Harold Conner Jr.***

4:25 Paper 400c: Overcoming Challenges in First-Ever Demolition of a Gaseous Diffusion Complex — ***Kenneth Rueter***

4:55 Paper 400d: First Ever Nuclear Decommissioning Minor in U.S. — ***Wesley Hines***

5:25 Paper 400e: Nuclear Facilities Operations Expertise at the Savannah River Site and the Lawrence Livermore Laboratory — ***Howard Walls Sr.***

5:50: Panel Discussion

(401) AIChE Inorganic Materials Graduate Student Award, Sponsored by Chevron

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-122A

Kumar Varoon Agrawal, Chair
Satish Nune, Co-Chair

Sponsored by: Inorganic Materials

3:30 Paper 401a: Development of Coarse-Grained (CG) Embedded Atom Method (EAM) Potentials for FCC Metals Using Machine Learning and Bayesian Uncertainty Quantification — ***Abhishek Sose***, *Troy Gustke, Fangxi Wang, Aditya Savara, Sanket Deshmukh*

3:50 Paper 401b: Beyond Interfacial Resistance: Interface Design for Dendrite-Free All-Solid-State Lithium Metal Batteries — ***Xinzi He***, *Chunsheng Wang*

4:10 Paper 401c: High-Throughput Computational Screening of Mxene for CO_2 Capture from Syngas and the Effect of Interlayer Distance on Ideal Gas Separation — ***Sirin Massoumilari***, *Sadiye Velioglu*

4:30: Break

4:50 Paper 401e: Engineering Zeolite Syntheses with Inorganic Structure-Directing Agents — ***Adam J. Mallette***, *Aseem Chawla, Rishabh Jain, Nathan Varghese, Francisco C. Robles Hernández, Jeffrey Rimer*

5:10 Paper 401f: Structure and Transport Studies of Carbon Molecular Sieve Membranes for Wastewater Treatment — ***Young Hee Yoon***, *Daniel O'Nolan, Michelle Beauvais, Karena Chapman, Ryan P. Lively*

5:30 Paper 401g: A Mechanism Study on the Incorporation of Vacancy Defects in Graphene Lattice By Oxidative Etching — ***Shaoxian Li***, *Tohidi Vahdat Mohammad, Shiqi Huang, Nicola Marzari, Kumar Varoon Agrawal*

(402) Biomimetic Materials II

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-121C

Xi Chen, Chair
Bret Ulery, Co-Chair
Yifan Cheng, Co-Chair
Christina Bailey-Hytholt, Co-Chair

Sponsored by: Biomaterials

3:30 Paper 402a: Exploring Actin Network Mechanics Via Synthetic Bio-Hybrid Crosslinkers — ***Tyler Jorgenson***, *Margaret L. Gardel, Stuart J. Rowan*

3:48 Paper 402b: Multiscale out-of-Equilibrium Structural Evolution in Bio-Based Composites — ***John Berezney***, *Seth Fraden, Zvonimir Dogic*

4:06 Paper 402c: Integration of Cell-Free Protein Expression with Recombinant Fusion Protein Assemblies — ***Jackson Powers***, *Yeongseon Jang, Seok Hoon Hong*

4:24 Paper 402d: Preparation of Structured Bio-Inspired Composite Materials through Magnetic Control of Sol-Gel Phase Transitions — ***Marco Lattuada***

4:42 Paper 402e: Peptidoglycan-Bioconjugates from Extremophillic Microorganisms for New Bioinspired Water-Responsive Materials — ***Malcolm Lane Gilchrist***, *Seungri Kim, Xi Chen*

5:00 Paper 402f: Proteoliposome Development for Placental Biomimetic Models — ***Daniel Zimmer***, *Christina Bailey-Hytholt*

5:18 Paper 402g: Surfaces with antifouling-antimicrobial dual function *via* immobilization of lysozyme on zwitterionic polymer thin films — ***Alexandra Khlyustova***, *Mia Kirsch, Xiaojing Ma, Yifan Cheng, Rong Yang*

5:36 Paper 402h: Controlling the Properties of the Light-Responsive Transmembrane Protein Proteorhodopsin in Mesostructured Silica-Surfactant Hybrid Materials — ***Maxwell Berkow***, *Songi Han, Bradley F. Chmelka*

(403) Charged and Ion Containing Polymers III

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-121A

Allie Obermeyer, Chair
Hee Jeung Oh, Co-Chair
Chibueze Amanchukwu, Co-Chair
Christian Aponte-Rivera, Co-Chair

Sponsored by: Polymers

3:30 Paper 403a: Unifying Weak and Strong Charge Correlations within the Random Phase Approximation for Sequence-Defined Polyampholytes — ***Artem Rumyantsev***, *Albert Johner, Matthew V. Tirrell, Juan J. de Pablo*

3:45 Paper 403b: Molecular Dynamics Simulations of Single-Ion Block Copolymers: Effect of Polymer Architecture — ***Mengdi Fan***, *Lisa Hall*

4:00 Paper 403c: Hybrid Field Theory and Particle Simulation Model of Polyelectrolyte–Surfactant Coacervation — ***Jason Madinya***, *Charles Sing*

4:15 Paper 403d: Complex Coacervation in Polyelectrolyte Brushes — ***Christopher Balzer***, *Zhen-Gang Wang*

4:30 Paper 403e: Coarse-Grained Molecular Dynamics Simulation of Phase Behavior in Poly(styrene)-Block-Poly(ethylene glycol)/1-Ethyl-3-Methylimidazolium Thiocyanate Mixtures — ***Azam Salmankhani***, *Paul Scovazzo, Alexander Lopez, Adam Smith,* ***Sasan Nouranian***

4:45 Paper 403f: Constraint Release in Entangled Liquid Coacervates Made from Oppositely Charged Polyelectrolytes — ***Christian Aponte-Rivera***, *Michael Rubinstein*

5:00 Paper 403g: Modeling the Complexation of Homologous Polyelectrolytes — ***Jian Qin***

5:30 Paper 403h: Uptake Selectivity of Nanoparticles with Patterned Surface Charges in Sequence Controlled Polyampholyte Coacervates — ***Heyi Liang***, *Artem Rumyantsev, Juan J. de Pablo*

5:45 Paper 403i: Influence of Water Content on Ion Transport Properties of Highly Charged Ion Exchange Membranes for Vanadium Redox Flow Batteries — ***Gregory Reimonn***, *Jovan Kamcev*

(404) Excellence in Graduate Student Research (Area 08A)

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-121B

Danielle Mai, Chair
Ralm Ricarte, Co-Chair

Sponsored by: Polymers

3:30 Paper 404a: Nanoporous Membranes with Narrowed Pore Size Distribution Via *Initiated* Chemical Vapor Deposition — ***Alexandra Khlyustova***, *Yifan Cheng, Rong Yang*

3:45 Paper 404b: Modeling Local pH and Ionic Fluxes in Bipolar Membranes — ***Justin Bui***, *Alexis T. Bell, Adam Weber*

4:00 Paper 404c: The Modular Design of Charge Transport in Radical Polymers — ***Ying Tan***, *Bryan Boudouris, Brett Savoie*

4:15 Paper 404d: Taking a Metal–Ligand Coordination Approach Towards High Ionic Conductivity Ca–Polymer Electrolytes — ***Shreyas Pathreeker***, *Ian Hosein*

4:30 Paper 404e: Expanding the Toolbox of Living Branching Polymerization through Simulation-Informed Reaction Design — ***Mengxue Cao***, *Mingjiang Zhong*

4:45 Paper 404f: A Molecular Design Approach Towards Elastic and Multifunctional Polymer Electronics — ***Yu Zheng***, *Zhenan Bao*

5:00 Paper 404g: Resorcinol-Added Phenolic Resins for Carbon/Carbon Composite Fabrication: Kinetics for Curing Prediction and Application — ***Jose Cordeiro Jr.***, *Rachel Davis, Hema Ramsurn, Daniel W. Crunkleton, Todd Otanicar, Michael Keller*

5:15 Paper 404h: Evaluation of UV-Curable Polymeric Binders for Additive Manufacturing Construction in Space Environments — ***Alexandra Marnot***, *Blair Brettmann*

5:30 Paper 404i: Understanding Creep Suppression Mechanism in Polymer Nanocomposites through Machine Learning — ***Entao Yang***, *James Pressly, Bharath Natarajan, Robert Colby, Karen Winey, Robert Riggleman*

5:45 Paper 404j: Predicting Viscoelasticity of Dynamically Associating Polymer Networks Using Brachiation Theory — ***Pamela Cai***, *Matthew Webber, Sarah Heilshorn, Andrew Spakowitz*

(405) Polymer Networks and Gels I

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-122B

Kenneth Mineart, Chair
Jinhye Bae, Co-Chair
Xiaoguang Wang, Co-Chair

Sponsored by: Polymers

3:30 Paper 405a: Highly Stretchable Hydrogels and Their Retraction Behavior — ***Santanu Kundu***, *Anandavalli Varadarajan, Rosa Maria Badani Prado, Satish Mishra*

4:00 Paper 405b: Heat and Acid-Induced Hydrogels from Soybean Hull: Effect of Processing Conditions — ***Navid Etebari Alamdari***, *Burak Aksoy, Zhihua Jiang*

4:15: Break

4:30 Paper 405d: Influence of Polymerization Conditions on Collagen I, II, and III Blend Hydrogels — *Paulina Babiak,* ***Carly Battistoni***, *Leonard Cahya, Jason Minnich II, Rithika Athreya, Alyssa Panitch, Julie C. Liu*

4:45 Paper 405e: Performance of a Commercial Preformed Particle Gels (PPGs) in High Temperature and Saline Medium — *Ahmed Ben Ali, Reem Elaf,* ***Ibnelwaleed Hussein***, *Mohammed Ali Saleh, Baojun Bai*

5:00 Paper 405f: Development of Novel Crosslinked Polymer Gel Composite As Lost Circulation Materials for Oil and Gas Wells — *Ahmed Hamza, Mohamed Shamlooh,* ***Mustafa Nasser***, *Ibnelwaleed Hussein*

5:15 Paper 405g: The Effect of Crosslinker Concentration on Drug Release Kinetics of Thermo-Responsive, Lignin-Based Soft Composites — ***Missoury Lytle***, *Alana LeSuer, Graham W. Tindall, Mark C. Thies, Eric M. Davis*

5:30 Paper 405h: Biocatalytic 3D Actuation in Liquid Crystal Elastomers Via Enzyme Patterning — ***Albert Velasco Abadia***

5:45 Paper 405i: Liquid Crystal Elastomeric Nanowires — ***Xiaoguang Wang***, *Robert Dupont, Yang Xu*

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(406) Experimental Investigations of Mixing Processes

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-227C

Thomas A. Simpson, Chair
Emilio Tozzi, Co-Chair

Sponsored by: North American Mixing Forum

3:30 Paper 406a: Development of Turbulence Measurement Technique Using Electrical Resistance Tomography for Multiphase Flows — ***Weiguo Xie***

3:55 Paper 406b: Power, Flow and Efficiency: Effect of Adding Tiplets on Impeller Efficiency — ***Richard Grenville***, *Jason Giacomelli, Benjamin Boyer, Bernd Gigas*

4:20 Paper 406c: Hydrodynamics Investigation of the USP Dissolution Testing Apparatus 1 (Basket Apparatus) Filled with 500 Ml Media Volume Using Particle Image Velocimetry (PIV) — ***Chadakarn Sirasitthichoke***, *Piero Armenante*

4:45 Paper 406d: Application of a Combined PIV/PTV-Method to Analyze Suspensions in (non-)Newtonian Media in Stirred Tanks — ***Markus Kolano***, *Matthias Kraume*

5:10: Break

5:35 Paper 406f: Experimental Investigation on the Power Input of Viscoelastic Fluids in an Unbaffled Tank — ***Alexander Maywurm***, *Lutz Böhm, Matthias Kraume*

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(407) Engineered Particles and Nanostructured Particulate Systems Characterization

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, W-106C

Jung-Sheng Wu, Chair
Sheena Reeves, Co-Chair
Mohammad Azad, Co-Chair

Sponsored by: Particle Production and Characterization

3:30: Break

3:50 Paper 407b: Crystal Growth Impedance from Boundary Layer Transport, Conformational Interconversion, and Dimerization Kinetics — ***Armin Shayesteh Zadeh***, *Baron Peters*

4:10 Paper 407c: Direct Ink Writing of Tungsten and Tungsten Alloys for Dense Complex Shapes — ***Hailey Loehde-Woolard***, *Elena Napoletano, Davis R. Conklin, Bergen Evans, James Smay, Alan Weimer*

4:30 Paper 407d: Adapting Cold Spray Technology to Polymer Powders — ***Tristan Bacha***, *David A. Brennan, Anuraag Gangineri Padmanaban, Jae-Hwang Lee, Francis M. Haas, Joseph F. Stanzione III*

4:50 Paper 407e: 3D-Printing Hybrid Electrolyte Structures for Dendrite Suppressions — ***Nathan Fonseca***

5:10 Paper 334c: Synthesis and Characterization of Aluminum Boride Particles Coated with Plasma Nanofilms for Energetic Applications — ***Prawal P. K. Agarwal***, *Themis Matsoukas*

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(408) Particle Technology in Product Design and Manufacturing

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, W-106A

Jorg Theuerkauf, Chair
Kensaku Matsunami, Co-Chair

Sponsored by: Solids Flow, Handling and Processing

3:30 Paper 408a: Development of an Online Free Web Application to Perform Multivariate Analysis and Determine Microcrystalline Cellulose Crystallinity from Raman Spectra — ***Ana L. P. Queiroz***, *Abina Crean*

3:48 Paper 408b: Influence of the Feed Frame Design on a Continuous Manufacturing Process — ***Peter Boehling***, *Johan Remmelgas, Julia Kruisz, Johannes Poms, Manel Bautista, Johannes G. Khinast, Emmanuela Gavi*

4:06 Paper 408c: Using Multi-Level Coarse-Grained Simulation for Design Studies: The Case of Tablet Press Feeder — *Lokeshwar Mahto, Tarun De,* ***Jayanta Chakraborty***, *Jitendra Kumar, Anurag Tripathi, William Ketterhagen, Maitraye Sen, Krishnendu Basak*

4:24 Paper 408d: First Steps Toward Large-Scale Production of PLGA Nanoparticles — ***Carolin Tetyczka***, *Ramona Jeitler, Lukas Vergeiner, Daniela Fiedler, Dagmar Kolb, Gerd Leitinger, Eva Roblegg*

4:42 Paper 408e: Improving the Stability of Nuclear Thermal Propulsion Fuel Elements with Tungsten Atomic Layer Deposition — ***Davis R. Conklin***, *Sarah Bull, Christopher G. McKinney, Jamelle K.P. Williams, Arne Croell, Jhonathan Rosales, Alan Weimer*

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(409) Powder and Particulate Characterization and Measurement

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, W-106B

Parind Desai, Chair
Madhusudhan Kodam, Co-Chair

Sponsored by: Solids Flow, Handling and Processing

3:30: Introductory Remarks

3:48 Paper 409b: Packing Dynamics of Polymer Powders at High Temperature — ***Salvatore Pillitteri***, *Filip Francqui, Aurelien Neveu, Geoffroy Lumay*

4:06 Paper 409c: A Revolutionary, Evolutionary Approach to the Characterisation of Particulate Media: From Bulk Measurements to Micromechanical Properties — ***Kit Windows-Yule***

4:24 Paper 409d: Shear-Induced Dilation of Constrained Consolidated Powder Beds — *Tony Thornton, Katrina Brockbank, Jamie Clayton,* ***Amalia Thomas***

4:42: Break

5:00 Paper 409f: Flowability Measurements and Rheological Investigations of Volcaniclastic Debris Flows from Campania Plain (southern Italy) — ***Ilaria Rucco***, *Chongqiang Zhu, Fabio Dioguardi, Lyes Ait Ali Yahia, Lizeth Caballero, Mauro A. Di Vito, Damiano Sarocchi, Raffaella Ocone*

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(410) Continuous Processing in Drug Substance and Drug Product: Integrated Processes

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-123

Jasmine Rowe, Chair
Travis Armiger, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

3:30 Paper 410a: Risk Considerations on Developing a Continuous Synthesis and Crystallization Platform for Carbamazepine — ***Wei Wu***, *Matthew Glace, Adil Mohammad*

3:51 Paper 410b: Combining Reaction with Crystallization and a Size-Based Biocatalyst Separation for the Continuous Manufacturing of Amoxicillin — ***Patrick Harris***, *Hossein Salami, Colton Lagerman, Ronald Rousseau, Martha Grover, Andreas Bommarius*

4:12 Paper 410c: Moisture Content Monitoring in Continuous Drug Substance Isolation Manufacturing Platform — ***Inyoung Hur***, *Daniel Casas Orozco, Zoltan Nagy*

4:33 Paper 410d: Design of a Pilot Plant for Integrated Continuous Manufacturing of a Steroid API — ***Guanghui Zhu***, *Andriy Neshchadin, Zachary Fejedelem, Janaka Gamekkanda, Ahmet Aloglu, Sean Keenan, Stephen Born, Chuntian Hu*

4:54 Paper 410e: Continuous Twin-Screw Wet Granulation and Fluid-Bed Drying at the Pilot Scale and Comparison to Batch Granulation and Drying — ***Seth Forster***, *Erin Dippold, Abbe Haser, Imre Homolya, Daniel Emanuele, Robin Meier*

5:15 Paper 410f: Developing a Process Analytical Technology for Particle Size Determination in Twin Screw Granulation Using Acoustic Emissions — ***Hassan Abdulhussain***, *Michael R. Thompson*

5:36 Paper 410g: Computational Modeling of the Residence Time Distribution of Twin Screw Extrusion for Continuous Manufacturing Applications — ***Nisha Raman***, *William Blincoe, Morgan Giles, Nathan Rudd, Athanas Koynov*

(411) Integrated Product and Process Design with Pharmaceutical Applications II

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-122C

Pablo A. Rolandi, Chair
Qinglin Su, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

3:30 Paper 411a: Plug-and-Play Software for Mechanistic Modelling of End-to-End Continuous Manufacturing of Monoclonal Antibodies — ***Moo Sun Hong***, *Amos E. Lu, Richard D. Braatz*

3:51 Paper 411b: An Optimization-Based Approach to Identify Thermodynamically Stable Blends for Spray Drying Dispersions — ***Suela Jonuzaj***, *Malak Wehbe, Christopher Burcham, Amparo Galindo, George Jackson, Claire Adjiman*

4:12 Paper 411c: Impact of Excipient Properties & Blending Process Parameter on Blend Uniformity of a Blend Prepared in Small Batches Semicontinuously Using Integrated Feeder-Blender System — ***Sumit Kumar***, *Gintaras V. Reklaitis, Zoltan Nagy, Marcial Gonzalez, Paul R. Mort*

4:33 Paper 411d: Molecular Dynamics Modeling Based Investigation of the Effect of Freezing Rate on Protein Stability — ***Tibo Duran***, *Bruna Minatovicz, Ryan Bellucci, Jun Bai, Bodhisattwa Chaudhuri*

4:54 Paper 411e: A Multi-Scale Approach to Understanding Spray Dried Dispersion Impurity Generation — ***James Miesle***, *Salvador Garcia Munoz, Matthew Walworth, Jason Melnick, Lars Magnusson, Alana Kurz, Kerri Fischer*

5:15 Paper 411f: Parallel Process Development and Enzyme Evolution for Drug Substance Manufacturing — ***Sean Dubina***, *Scott McCann, Birgit Kosjek, Stephanie Chun, Nilusha Padivitage, Daniel DiRocco, Jonathan McMullen*

5:36 Paper 411g: An Industrial in silico Modeling Platform for Reliable, Efficient, and Agile Process & Product Development — ***Fabrice Schlegel***, *Pablo A. Rolandi, Iman Mirzaee, Maxwell Maritato, Saman Seifi, Miguel Angel Valderrama-Gomez, Joao De Faria, Saeed Jafari Kang, Maryam Medghalchi, Elcin Icten Gencer, Justin Porth*

(412) Process Intensification – Novel Integration Concepts

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-222A

Patrick Heider, Chair
Pranav Karanjkar, Co-Chair

Sponsored by: Process Intensification & Microprocess Engineering

3:30 Paper 412a: Kinetics and Spectroscopic Probes of the Surface Structure of Bi_2O_3 As a Selective Hydrogen Combustion Catalyst — ***Matthew Jacob***, *Aditya Bhan*

3:55 Paper 412b: High-Temperature, High-Pressure Reactions of Sulfur with Hydrocarbons: A Lab-Scale Experimental Study — *Peter Koronaios, Riddhesh Patel, Hseen Baled, Goetz Veser, Ryan Weber, Nicolas Proust, Josh Harntraft, Glenn Cormack,* ***Robert Enick***

4:20 Paper 412c: Reduction of the Generated Sugarcane Stillage in Distillation through HEAT Integration — ***Gianpaolo Barci***, *Paulo S. Barci, Murilo Innocentini*

4:45 Paper 412d: Process Intensification for Continuous Metal Extraction from E-Waste: Challenges and Opportunities — ***Jogender Singh***, *Aaliya Javed*

(413) Engineering Geologic Carbon Dioxide Storage Systems

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-226A

Kanwal Mahajan, Chair
Dawn Deel, Co-Chair
Melissa D'Andrea, Co-Chair

Sponsored by: Sustainable Energy

3:30 Paper 413a: Wyoming Carbonsafe: Accelerating Commercial Deployment of Carbon Capture and Storage in Wyoming. — ***Scott Austin Quillinan***, *Jonathan 'Fred' McLaughlin, Kipp Coddington, Zunsheng Jiao, Erin Phillips, Matthew Johnson, Davin Bagdonas, Ying Yu, Selena Gerace, Robert Gregory*

3:45 Paper 413b: Stacked Storage: Technical Considerations and Examples of Potential Reservoirs — ***Matthew Belobraydic***, *Nicholas Bosshart, John A. Hamling, James A. Sorensen*

4:00 Paper 413c: Overview of the UIC Class VI Permit Application for San Juan Basin Carbonsafe Phase III Project — ***Sai Wang***, *William Ampomah, George El-Kaseeh, Candace Candy, Richard Esser*

4:15 Paper 413d: Building the Permit for the First Carbon Storage Hub in the United States — ***David Riestenberg***, *George J. Koperna Jr., Richard Esposito, Kimberly Gray*

4:30 Paper 413e: North Dakota Carbonsafe – a Success Story — ***Wesley Peck***, *Kevin Connors*

4:45 Paper 413f: *On the Feasibility of Geophysical Methods for CO2 Monitoring in the North Dakota Carbonsafe Project* — ***Donald Adams***, *Cesar Barajas-Olalde, Kurt Stract, Sofia Davydycheva, Yardenia Martinez, Kris Maclennan, Ryan J. Klapperich, Wesley Peck, Shannon Mikula*

5:00 Paper 413g: CO_2 Adsorption in Partially Water-Saturated Kaolinite Nanopores from Molecular Perspectives in Relation to Geological Carbon Sequestration — *Mingshan Zhang,* ***Zhehui Jin***

5:15 Paper 413h: Evaluating CO_2 Hydrate Stability in Oceanic Sediments for CO_2 Sequestration — ***M Fahed Qureshi***, *Vikas Dhamu, Adam Usadi, Timothy Barckholtz, Ashish B. Mhadeshwar, Praveen Linga*

(414) Feedstock Logistics for Biorefineries

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-226B

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

Sponsored by: Sustainable Biorefineries

3:30 Paper 414a: Transforming Biomass and Waste into Conversion-Ready Feedstocks for a Circular Carbon Economy — ***Lynn Wendt***

3:51 Paper 414b: Ivory Nut *(Phytelephas equatorialis)* Residues: Chemical Composition for Applications in Health Care, Industry and Environmental Remediation - Towards Sustainabilty — ***Lourdes Orejuela Escobar***, *Ana Andrade, Christian Luciani, Dario Niebieskikwiat*

4:12 Paper 414c: Removing Selective Structural Inorganics from Corn Stover By Type III Deep Eutectic Solvent — ***Md Tahmid Islam***, *Laura Guidugli, Jordan Klinger, Toufiq Reza*

(415) Fuel and Energy Decarbonization

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-226C

Eric Tan, Chair
William Barrett, Co-Chair

Sponsored by: Sustainable Energy

3:30 Paper 415a: Ammonia and Methanol As Sustainable Energy Storage Vectors: A Techno-Economic and Environmental Comparative Analysis — ***Sebastiano C. D'Angelo***, *Michael Bregy, Philipp Steiner, Raul Calvo-Serrano, Gonzalo Guillén-Gosálbez*

3:42 Paper 415b: Waste Heat Recovery Using Thermochemical Energy Storage — ***Fuqiong Lei***, *Irene Walker, Alpha Toure, Nick AuYeung*

3:54 Paper 415c: Dynamic Life-Cycle Analysis of Short-Lived Greenhouse Gases: Paving the Way for Improved Policy and Decision-Making — ***Santiago Salas***, *Qining Chen, Kirsten Rosselot, Jennifer B. Dunn, David Allen*

4:06 Paper 415d: Thermo-Catalytic Decomposition of Decarbonization of Natural Gas — *Mpila Nkiawete,* ***Randall Vander Wal***

4:18 Paper 415e: Green-Hydrogen Production: Systematic Superstructure-Based Approach for Technology Selection — ***Mariana Corengia***, *Ana I. Torres*

4:30 Paper 415f: Role of Fuels in Decarbonization and Energy Transition — ***Praveen Cheekatamarla***

4:42 Paper 415g: Experimental Evaluation of Catalytic Transients Involved in Reservoir Natural Gas Reforming — *Rahman Gholami, Roman Berenblyum, Klaus Hellgardt,* ***Lu Ai***

4:54 Paper 415h: Leveraging Photons for Sustainable Catalysis and Energy Production: From Bench to Industry — ***Hossein Robatjazi***

5:06 Paper 415i: Numerical Modeling of Chemical Looping Oxidative Dehydrogenation of Ethane in a Packed Bed Reactor — ***Runxia Cai***, *Leo Brody, Yuan Tian, Luke Neal, Arnab Bose, Fanxing Li*

5:18 Paper 415j: Electrochemical Conversion of CO2 from Flue Gas on Sn-Coated Cu2O Nanoparticles — *Subhajyoti Samanta, Marcello Ferrara, Paolo Fornasiero,* ***Jonas Baltrusaitis***

5:30 Paper 415k: A Conceptual Design of an Allam-Cycle Centered Industrial Complex for CO_2 Enhanced Oil Recovery — ***Ying Liu***, *Qiang Xu*

5:42 Paper 415l: Strain Effects on Oxygen Binding and Phase Change on Pd Surfaces — ***Trenton Wolter***, *Matteo Cargnello, Manos Mavrikakis*

(416) Innovations in Methods of Data Science

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-125A

Shuwen Yue, Chair
Srinivas Rangarajan, Co-Chair
Curtis Martin, Co-Chair

Sponsored by: Applications of Data Science to Molecules and Materials

3:30: Introductory Remarks

3:31 Paper 416a: Global Systems Analysis Using Deep Learning on Industrially Relevant Large Datasets — ***Gurkan Sin***, *Adem Rosenkvist Nielsen Aouichaoui*

3:47 Paper 416b: Uncertainty Quantification for Molecular Property Predictions Using Automatic Graph Neural Architecture Search — ***Shengli Jiang***, *Shiyi Qin, Prasanna Balaprakash, Reid Van Lehn, Victor Zavala*

4:03 Paper 416c: Projecting the Effectiveness of Deep Ensembles — ***Charles McGill***, *William Green*

4:19 Paper 416d: Automatic Strain Sensor Design *Via* Active Learning and Data Argumentation for Soft Machines — ***Po-Yen Chen***, *Tianle Chen*

4:35 Paper 416e: A Framework for the Statistical Value of Extreme Points for Function Approximation — ***Arijit Chakraborty***, *Krishnan Kumaran, Venkat Venkatasubramanian*

4:51: Break

4:56 Paper 416f: Graph Hysteria – Comparing the Generative Performance of Graph and String-Based Translation Vaes for Molecular Design — ***Orion Dollar***, *Nisarg Joshi, David Beck, Jim Pfaendtner*

5:12 Paper 416g: Extending Bigsmiles to Non-Covalent Bonds in Supramolecular Polymer Assemblies — ***Weizhong Zou***, *Alexis Martell-Monterroza, Yunxin Yao, S. Cem Milik, Morgan Cencer, Nathan Rebello, Haley Beech, Melody Morris, Tzyy-Shyang Lin, Cleotilde Castano, Julia Kalow, Stephen Craig, Alshakim Nelson, Jeffrey Moore, Bradley Olsen*

5:28 Paper 416h: Formal Proofs in the Chemical Sciences Using the Lean Theorem Prover — ***Parivash Feyzishendi***, *Maxwell P. Bobbin, Catherine M. Wraback, Samiha Sharlin, Tyler R. Josephson*

5:44 Paper 416i: Machine Learning with Differential Equation Priors — ***Aditi Krishnapriyan***

(417) Infection & Prevention, Epidemiology & Treatments, Diagnostic Approaches

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-126C

Leonard Pease, Chair
Swomitra Mohanty, Co-Chair

Sponsored by: Chemical Engineers in Medicine

3:30 Paper 417a: Two Complementary Memory B Cell Processes Generate Antibody Protection Against the Same or Variant Viruses — ***Matthew Vanbeek***

3:49 Paper 417b: A Model for How T Cell-Mediated Autoimmunity Can be Triggered By Persistent Viral Infections — ***Rose Yin***, *Samuel Melton, Eric Huseby, Mehran Kardar, Arup K. Chakraborty*

4:08 Paper 417c: Predicting the Effects of Sars-Cov-2 Spike Protein Mutations to MHC Class II – Mediated Immune Responses — ***Mercedes Haley***, *Sumaiya Islam, Robert Pantazes*

4:27 Paper 417d: Inhibition of Sars-Cov-2 Spike Protein Pseudotyped Virus Infection Using ACE2-Tethered Micro/Nanoparticles — ***Soha Alkhaldi***, *Ian Peng, Esmael Alyami, Ammar Ahmad Tarar, Ching-An Peng*

4:46 Paper 417e: A Novel SERS-Based Assay for Detection of the Sars-Cov-2 Spike Protein — ***Karen Wawrousek***, *Moein Mohammadi, Delphine Antoine, Madison Vitt, Sharmin Sultana Jyoti, Julia Dickie, Gerard Wall, Patrick A. Johnson*

5:05 Paper 417f: Cell-Free, Dendritic Cell-Mimicking Vaccines for Cancer, COVID-19, and Beyond — ***Melissa N. Thone***, *Jee Young Chung, Young Jik Kwon*

5:24 Paper 417g: Agent-Based Modeling of Sars-Cov-2 Transmission during the COVID-19 Pandemic at the University of Delaware — *Soham Jariwala, **Norman J. Wagner**, Antony Beris, Richard Suminski, Gregory Dominick*

(418) Interfacial Systems for Energy Application: Modeling and Simulation

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-227A

Gyeong Hwang, Chair
Alan Weimer, Co-Chair

Sponsored by: Material Interfaces as Energy Solutions

3:30 Paper 418a: Computationally Guided Discovery of Mixed Mn/Ni Perovskites for Solar Thermochemical Hydrogen Production at High H_2 Conversion — ***Ryan Morelock**, Justin Tran, Zachary Bare, Jamie Trindell, Anthony H. McDaniel, Alan Weimer, Charles B. Musgrave*

3:48 Paper 418b: Understanding the Nanostructure and Performance of Alumina Atomic Layer Deposited Films on a Layered Cathode Oxide Surface Using Molecular Dynamics Simulation — ***Julie A. Nguyen**, Abigayle Becker, Krishan Kanhaiya, Alan Weimer, Hendrik Heinz*

4:06 Paper 418c: First-Principles Modeling of Discharge Product Surface Thermodynamics in Na-O_2 Batteries — ***Alex Von Gunten**, Kunal Velinkar, Eranda Nikolla, Jeffrey Greeley*

4:24 Paper 418d: Interfacial Stability of Al and Ga Dopants at the Lithium Garnet | Lithium Metal Interface — ***Matthew Klenk**, Michael Counihan, Zachary Hood, Justin Connell, Sanja Tepavcevic, Peter Zapol*

4:42: Break

5:00 Paper 418f: Synergistic Effects between Geometric and Electronic Factors on Crystallized Polymer-Coated Pt Catalyst for Hydrogen Evolution Reaction — ***Chi-Ho Lee**, Jung-Hyun Park, Hong Yang, Joseph Kwon*

5:18 Paper 418g: Insights into the Effects of Micropore Structure and Electrolyte Composition on the Energy Storage Performance of Electrical Double Layer Capacitors — ***Betul Uralcan***

5:36 Paper 418h: Molecular Insights on the Performance of Nanoporous Carbide-Derived Carbon Supercapacitors with Various Electrolytes — ***Xiaobo Lin**, Shern Tee, Peter Cummings*

(419) Cybersecurity and High-Performance Computing in Next-Gen Manufacturing

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-221B

Helen Durand, Chair
Joseph Kwon, Co-Chair

Sponsored by: Next-Gen Manufacturing

3:30 Paper 419a: Keynote Talk-on the Role of Control System Design on Detecting Cyberattacks — ***Matthew Ellis**, Shilpa Narasimhan, Nael El-Farra*

4:00 Paper 419b: Keynote Talk - Cybersecurity for Operational Technology and Smart Manufacturing Systems — ***CheeYee Tang***

4:30 Paper 419c: Safe Control of Networked Chemical Process Plants Under Cyber-Attacks — ***Jaewon Kim**, Akshay Mete, P. R. Kumar*

4:48 Paper 419d: Lyapunov-Based Economic Model Predictive Control with Cyberattack Detection for Process Actuators — ***Keshav Kasturi Rangan**, Henrique Oyama, Helen Durand*

5:06 Paper 419e: Switching-Enabled Active Detection of False-Data Injection Cyberattacks on Process Control Systems — ***Shilpa Narasimhan**, Nael El-Farra, Matthew Ellis*

5:24 Paper 419f: Modeling Impacts of Cyberattacks on Control of Powder Bed Fusion — ***Kip Nieman**, Helen Durand*

5:42 Paper 419g: Limitations of Control-Theoretic Control System Cyberattack Detection for Distributed Control Leading to Cost/Benefit Analysis for Control System Cybersecurity — ***Dominic Messina**, Katrina Hinzman, Helen Durand*

(420) Modeling, Optimization, and Control in Next-Gen Manufacturing II

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-221A

Saurabh Maduskar, Chair
Amir Barati Farimani, Co-Chair
Q. Peter He, Co-Chair

Sponsored by: Next-Gen Manufacturing

3:30 Paper 420a: Deep Model-Based Reinforcement Learning for Active Flow Control of Turbulent Couette Flow — ***Kevin Zeng**, Alec Linot, Michael Graham*

3:55 Paper 420b: Computational Method for Optimization of Micro-Structured Materials for Passive Cooling Applications — ***Andrew Cochrane**, Weston Ortiz, Rekha Rao*

4:20 Paper 420c: Determining Appropriate Input Perturbation for an Improved Intensified Design of Experiments Approach for System Identification of a Continuous Bioprocess — *Samardeepsingh Sarna, **Nikesh Patel**, Brandon Corbett, Chris McCready, Prashant Mhaskar*

4:45 Paper 420d: Evaluating Implementation Feasibility of Cyberattack Detection Strategies Based on Lyapunov-Based Economic Model Predictive Control — ***Dominic Messina**, Helen Durand*

5:10 Paper 420e: Ontology Engineering: Support to Decision Making in Biorefining — ***Franjo Cecelja**, Edlira Kalemi, Nikolaos Trokanas, Linsey Koo*

5:35 Paper 420f: Benchmarking Model Selection Criteria within an Automated Kinetic Rate Equation Discovery Framework — ***Miguel Ángel de Carvalho Servia**, Antonio del Rio Chanona, Dongda Zhang, Klaus Hellgardt, Mimi Hii*

(421) Sustainable Pathways to Clean Hydrogen and Synthetic Fuels III

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, W-103B

William Gibbons, Chair
Eric Miller, Co-Chair

Sponsored by: Sustainable Pathways Toward Hydrogen and Synthetic Fuels

3:30 Paper 421a: Economic Optimization of Grid-Integrated Clean Hydrogen and Ammonia Production — ***Matthew Palys**, Prodromos Daoutidis*

3:55 Paper 421b: Comparative Techno-Economic and Life Cycle Analysis of Conventional Ammonia with Carbon-Capture and Low-Carbon Hydrogen-Based Ammonia — ***Kyuha Lee**, Xinyu Liu, Pradeep Vyawahare, Pingping Sun, Amgad Elgowainy, Michael Wang*

4:20 Paper 421c: Techno-Economic Optimization of a Microwave-Assisted, Low-Pressure Ammonia Synthesis Process with Novel Separation Technologies — ***Opeyemi Ogunniyan**, Chirag Mevawala, Md Emdadul Haque, Yuxin Wang, Debangsu Bhattacharyya, Jianli Hu*

4:45 Paper 421d: Influence of Reductant Composition on NH_3 Synthesis from Exhaust NO Gas Using NO-CO-H_2O-H_2 Reaction — ***Anthony Hamzah**, Hideyuki Matsumoto, Yuichi Manaka, Tetsuya Nanba*

(422) Plenary Session: Waste Plastics (Invited Talks)

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-124AB

Jeffrey Seay, Chair
Shelby Browning, Co-Chair

Sponsored by: Waste Plastics

3:30 Paper 422a: Plastic Flows and Recycling Processes in the U.S.: Material Recovery Facilities and PET Processes — ***Raymond Smith***

4:00 Paper 422b: Prospective Issues on the Reuse of Plastics at the End-of-Life Stage in Europe — *Baibhaw Kumar, Natalia Cano, Felipe Moura, Gerardo Ruiz-Mercado,* ***Heriberto Cabezas****, Csaba Deak*

4:30 Paper 422c: Finding Strategic Solutions to Waste Plastics, Recycling and Beneficial Reuse Toward Circular Economy — ***Tapas K. Das****, Robert Peters*

5:00 Paper 422d: Global Plastic Pollution Policy Developments for Chemical Engineers — ***Mary Ellen Ternes***

5:30 Paper 422e: Enabling Micro-entrepreneurs to convert plastic waste to Polyfuel using Appropriate Technology — ***Shelby Browning***

(423) Advanced Electrochemical Storage

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-227B

Andrej Lenert, Chair
Haider Al-Rubaye, Co-Chair

Sponsored by: Transport and Energy Processes

3:30 Paper 423a: Degradation Kinetics of Sodium Superoxide in a Sodium-Oxygen Battery — ***Kwong Yu Chan****, Bin Qin, Chi-Ying Vanessa Li*

3:51 Paper 423b: Going Faster: Analytical Models for Predicting Cell Cycling Performance in Redox Flow Batteries — ***Bertrand J. Neyhouse****, Jonathan Lee, Fikile R. Brushett*

4:12 Paper 423c: Anode Lithium Plating Detection and Charging Rate Optimization in Lithium-Ion Batteries — ***Arun Muthukkumaran****, Raghunathan Rengaswamy*

(424) SBE's James E. Bailey Award Lecture

Tuesday, Nov 15, 6:15 PM
Phoenix Convention Center, North Ballroom 120D

Sponsored by: Awards Committee

(425) Biomass Conversion I: Hydrodeoxygenation

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, N-128A

Siddarth Krishna, Chair
Canan Sener, Co-Chair
Jennifer Lee, Co-Chair

Sponsored by: Catalysis

8:00 Paper 425a: Origin of Selective Tetrahydrofurfuryl Alcohol Ring Opening over Wox-Modified Pt(111), a DFT Study — ***Siddharth Deshpande****, Steven R. Denny, Sai Praneet Batchu, Zhexi Lin, William Porter, Dionisios Vlachos, Jingguang G. Chen, Stavros Caratzoulas*

8:18 Paper 425b: Identifying Effects of Phosphorous in Transition Metal Phosphides for Selective Hydrogenolysis of Hindered C–O Bonds — ***Conor Waldt****, David Hibbitts, Hansel Montalvo-Castro, Abdulrahman Almithn*

8:36 Paper 425c: Hydrodeoxygenation of Aliphatic Lignin Pyrolysis Vapors with Bulk MoO_3 — ***Andrew J. Kohler****, Brent H. Shanks*

8:54 Paper 425d: Screening of Novel Ni-Based Catalysts for Hydrodeoxygenation of Modelled Bio-Oils Using DFT — ***Seba AlAreeqi****, Daniel Bahamon, Kyriaki Polychronopoulou,* ***Lourdes Vega***

9:12 Paper 425e: Guaiacol Hydrodeoxygenation and Hydrogenation over Bimetallic Pt-M (Nb, W, Zr)/KIT-6 Catalysts with Tunable Acidity — ***Yang Xiao****, Anand Ramanathan, Bala Subramaniam, Arvind Varma*

9:30 Paper 425f: Enhancement in the Bio-Oil Hydrodeoxygenation Performance of Mo_2c Due to Tungsten Doping: A DFT Study Using Lignin and Carbohydrates Derived Model Compounds — ***Sagar Bathla****, Samir H. Mushrif*

9:48 Paper 425g: Elucidating the Role of Carbon in the Hydrodeoxygenation of Phenol in Iron Carbide-Based Catalysts — ***Neeru Chaudhary****, Renqin Zhang, Alyssa Hensley, Yong Wang, Jean-Sabin McEwen*

10:06 Paper 425h: Direct Deoxygenation Reaction of Biomass Pyrolysis Model Compounds on Ni_5P_4(001) Surface: Computational Study — *Omer Elfaki,* ***Kyriaki Polychronopoulou***

(426) Data Science & Machine Learning Approaches to Catalysis I: Interpretable and Theory-Guided Machine Learning For Catalysis Design and Understanding

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, N-128B

Bryan Goldsmith, Chair
Eric Walker, Co-Chair
Fanglin Che, Co-Chair

Sponsored by: Catalysis

8:00 Paper 426a: Opportunities for Symbolic Machine Learning and Automated Reasoning in Chemical Engineering — ***Tyler Josephson***

8:36 Paper 426b: Enhanced Descriptor Identification and Mechanic Understanding for Catalytic Activity with Data-Driven Framework: Revealing the Interactions between Elementary Steps — ***Wenjie Liao****, Ping Liu*

8:54 Paper 426c: Latent Variable Machine Learning Framework for Catalysis — ***Gbolade Kayode****, Chukwudi Nwaokorie, Matthew Montemore*

9:12 Paper 426d: Discovery of Pt Trimetallic Electrocatalysts for Ammonia Oxidation with Interpretable Deep Learning — ***Hemanth Pillai****, Yi Li, Shih-Han Wang, Qingmin Mu, Claire Pokrywka, Luke E. K. Achenie, Frank Abild-Pedersen, Gang Wu, Hongliang Xin*

9:30 Paper 426e: Dimensionality Reduction of Chemical Kinetics Based on Extent-of-Reaction in a Physics-Inspired Machine Learning Framework — ***Gabriel Gusmão****, Andrew Medford*

9:48 Paper 426f: An Electronic Descriptor Based Machine Learned Model for Adsorption Energies on Oxide Materials — ***Benjamin Comer****, Jiang Li Sr., Frank Abild-Pedersen, Michal Bajdich, Kirsten Winther*

10:06 Paper 426g: Maximum Entropy Inference in Chemical Reaction Networks with Unknown Kinetic Parameters — ***Mehrad Ansari****, Andrew White*

(427) Electrocatalysis I: Experimental and Theory

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, N-127C

Feng Jiao, Chair
Astrid Muller, Co-Chair
Huiyuan Zhu, Co-Chair

Sponsored by: Catalysis

8:00 Paper 427a: Descriptors for Anion Adsorption Energetics on Metal Electrodes — *Mohammad Hasibul Hasan,* ***Ian McCrum***

8:25 Paper 427b: Electrochemistry with Oxygen: New Design Principles for Next Generation Electrocatalysts — ***Michal Bajdich***

8:46 Paper 427c: Atomistic Simulations of Reaction Kinetics at Electrochemical Interface — ***Yuanyue Liu***

9:07 Paper 427e: Incorporating Electrode-Electrolyte Interfacial Effects on the Specific Adsorption of Ions on Late Transition Metal Surfaces Using a Combined DFT/FF-MD Approach — ***Andrew Wong****, Bolton Tran, Naveen Agrawal, Scott T. Milner, Michael J. Janik*

9:28 Paper 427f: Achieving Complete Electrooxidation of Ethanol By Single Atomic Rh Decoration of Pt Nanocubes — ***Qiaowan Chang****, Youngmin Hong, Hye Jin Lee, Ji Hoon Lee, Sang-Il Choi, Shyam Kattel, Zheng Chen, Jingguang G. Chen*

9:49 Paper 427g: Electrolyte Effects in Electrocatalytic Transformations — ***Nitish Govindarajan****, Karen Chan*

10:10 Paper 427h: Identifying the Stoichiometry of the Metastable Cu^{3+} State in Alkaline Electrochemical Systems — ***Lars Ostervold III****, Bolton Tran, Maxwell Wetherington, Konstantinos Alexopoulos, Michael J. Janik, Lauren F. Greenlee*

(428) Next Generation of CRE: a Professional Development Panel

Wednesday, Nov 16, 9:00 AM
Phoenix Convention Center, N-127A

Sheima Khatib, Chair

Sponsored by: Catalysis and Reaction Engineering Division

(429) Mid Career Researchers in Catalysis and Reaction Engineering Recognition Symposium (Invited Talks)

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, N-127B

Sheima J. Khatib, Chair
Andrew Medford, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

8:00 Paper 429a: Two Pulses Are Better Than One: Using Pump/Probe Dynamics to Deconvolve the Complexity of Properties and Pathways on Heterogeneous Catalysts — ***Rebecca Fushimi***

8:30 Paper 429b: C_2-C_4 Alkane/Alkene Diffusion and C_2-C_4 Alkene Methylation Reactions in Zeolites and Zeotypes Studied in TAP Experiments — ***Unni Olsbye***

8:50 Paper 429c: Insight into Carbon Gasification Via TAP — ***Vladimir Galvita***, *Hilde Poelman, Stavros Alexandros Theofanidis*

9:10 Paper 429d: Catalyst Design Strategies for Multifunctional Metal-Promoted Zeolites in the Conversion of Natural Gas to Aromatics — ***Sheima Khatib***

9:30 Paper 429e: Extracting Knowledge from Transient Kinetic Datasets — ***Andrew Medford***, *Adam Yonge*

9:50 Paper 429f: Transient Interplay of Catalytic Cycle and Deactivation — ***Gregory Yablonsky***, *Zoë Gromotka, Denis Constales, Nickolay Ostrovskii*

10:10 Paper 429g: Every Transient Tells a Story — ***John T. Gleaves***

(430) Modeling and Analysis of Chemical Reactors I

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, N-223

Anthony Dixon, Chair
Saurabh Bhandari, Co-Chair

Sponsored by: Reaction Engineering

8:00 Paper 430a: Scale-up Analysis of the Oxidative Dehydrogenation of Ethane over M1 Phase Catalysts in an Autothermal Reactor — ***Jiakang Chen***, *Praveen Bollini, Vemuri Balakotaiah*

8:18 Paper 430b: Optimization-Based Strategies for Spectral Analysis and Kinetic Modeling — ***Thomas Krumpolc***, *Daniel W. Trahan, Daniel Hickman, Xiaoyun (Shawn) Chen, Lorenz T. Biegler*

8:36: Intermission

8:54 Paper 430d: Computational Fluid Dynamics Simulation of Hydrodynamics in a Rotating Cylinder Electrode Reactor: Understanding Mass Transport Effects in Electrocatalysis — ***Derek Richard***, *Matthew Tom, Sungil Yun, Panagiotis Christofides, Carlos Morales-Guio*

9:12: Break

9:30 Paper 430f: Characterization of Stable Flow Conditions in Fixed Bed Reactors with Downwards Directed Flows — ***Gregor Wehinger***, ***Tanita Six***, *Niklas Paul, Armin Rix, Johannes Knossalla, Robert Franke*

9:48 Paper 430g: Novel Multiplicity and Stability Criteria for Polytropic Fixed-Bed Reactors — ***Jens Bremer***, *Kai Sundmacher*

10:06 Paper 430h: Multiobjective Optimization of Forced Periodic Operation of Methanol Synthesis — *Carsten Seidel, Johannes Leipold, Daliborka Nikolic,* ***Andreas Seidel-Morgenstern***, *Achim Kienle*

(431) Practical Applications of Computational Chemistry and Molecular Simulation for Complex Fluids and Phase Behavior

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, N-222B

Steven G. Arturo, Chair
Sukrit Mukhopadhyay, Co-Chair
Christopher Muhich, Co-Chair
Jonathan Moore, Co-Chair
Andrea R. Browning, Co-Chair
Martin Sanborn, Co-Chair
Mayank Agrawal, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

8:00 Paper 431a: A Quantitative, Molecular Simulations Based, Kinetic Model of Acid Gas Absorption in Aqueous Amines — ***Frederick de Meyer***, *Bénédicte Poulain, Xavier Rozanska*

8:30 Paper 431b: Accessible DPD Models for Structured Formulations Via Automated and Atomistically-Driven Parameterization — ***David A. Nicholson***, *John C. Shelley, Andrea R. Browning, Mayank Misra, Mohammad Atif Faiz Afzal, Paulo G. M. Mileo, H. Shaun Kwak, Mathew D. Halls*

8:50 Paper 431c: Multi-Scale Simulations Relevant for Hydrates Management — ***Alberto Striolo***, *Alberto Striolo*

9:10 Paper 431d: Progress Towards Alchemical Simulations Driven By Many-Body Gradient-Domain Machine Learning — ***Alex M. Maldonado***, *John Keith*

9:30 Paper 431e: Exploration of the Retention Mechanism in Supercritical Fluid Chromatography by Molecular Simulations — ***Chun-Kai Chang***, *Joern Siepmann, Faith L. Wroniuk, Yih Ling Saw, James P. Grinias, Mark R. Schure, Stephanie A. Schuster*

9:50 Paper 431f: Impacts of Surface Functionalization on the Cellulose Nanocrystal Solubility in Ethanol — ***Arash Elahi***, *Santanu Chaudhuri*

10:10 Paper 431g: Rational Design of Solvents for Catalytic Transformation of Biorenewable Platform Chemicals — ***Mohd Ussama***, *Gourav Shrivastav, M. Ali Haider*

(432) Advances in Machine Learning and Intelligent Systems I

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, W-101A

Qi Zhang, Chair
Seongmin Heo, Co-Chair

Sponsored by: Information Management and Intelligent Systems

8:00 Paper 432a: Learning-Based Estimation for Distributed Parameter Systems — ***Junyao Xie***, *Biao Huang, Stevan Dubljevic*

8:19 Paper 432b: Developing an LSTM-ANN Model for Prediction and Optimal Control of Kappa Number and Degree of Polymerization in a Batch Pulp Digester — ***Parth Shah***, *Hyun-Kyu Choi, Joseph Kwon*

8:38 Paper 432c: Lstm Neural Networks and Nonlinear State Space Model Identification — *Jicheng Li,* ***S. Joe Qin***

8:57 Paper 432d: Statistical Machine-Learning-Based Predictive Control of Nonlinear Time-Delay Processes — ***Aisha Alnajdi***, *Zhe Wu,* ***Scarlett (Siyao) Chen***, *Panagiotis Christofides*

9:16 Paper 432e: Fast Symbolic Regression with Constraints — ***Owais Sarwar***, *Nikolaos Sahinidis*

9:35 Paper 432f: A Kinetic Model-Based Transfer Learning Approach to Predicting Cell Line-Specific Metabolic Behavior in Biomanufacturing — ***Yen-An Lu***, *Meghan G. McCann, Wei-Shou Hu, Qi Zhang*

9:54 Paper 432g: Break the Trade-Off Relationship between Detection and Diagnosis Performance through Explainable Deep Learning — ***Kyojin Jang***, *Kes Pilario, Nayoung Lee, Il Moon, Jonggeol Na, Inkyu Lee*

10:13 Paper 432h: Demonstration of Closed-Loop Machine-Learning-Guided Experimental Platform for the Discovery of Novel Dye-like Compounds — ***Richard Canty***, *Brent Koscher, Matthew McDonald, Seung Kyun Ha, Klavs Jensen*

(433) Design and Operations Under Uncertainty - I

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, W-101C

Qi Zhang, Chair
Xunyuan Yin, Co-Chair

Sponsored by: Systems and Process Operations

8:00 Paper 433a: Systematic Methods for Explaining Stochastic Programming Solutions — ***Tushar Rathi***, *Rishabh Gupta, Qi Zhang*

8:22 Paper 433c: Insights into Nonconvex Robust Optimization for Chemical Engineering Applications — ***Tom Savage***, *Dongda Zhang, Antonio del Rio Chanona*

8:44 Paper 433d: Tighter Lower Bounds for Semi-Infinite Programming Using Parametric Sensitivity Theory — *Evren Turan, Johannes Jäschke,* ***Rohit Kannan***

9:06 Paper 433e: Stable Two-Stage Scenario Tree Generation Method Via a Game-Theoretic Optimization Approach — ***Georgios Bounitsis***, *Lazaros G. Papageorgiou, Vassilis Charitopoulos*

9:28 Paper 433f: Bounding Approaches to Various Multistage Stochastic Programming Problems with Type II Endogenous Uncertainty — ***Yasuhiro Shoji***, *Selen Cremaschi*

9:50 Paper 433g: A Multi-Scenario Stochastic Framework for Dynamic Real Time Optimization Under Uncertainty with Embedded Closed-Loop MPC — ***Lloyd MacKinnon***, *Christopher Swartz*

10:12 Paper 433h: Continuous Multi-Fidelity Bayesian Optimization for Efficient Integrated Process Design and Advanced Control — ***Farshud Sorourifar***, *Joel Paulson*

(434) Estimation and Control under Uncertainty

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, W-101B

Jin Wang, Chair
Davood Babaei Pourkargar, Co-Chair

Sponsored by: Systems and Process Control

8:00 Paper 434a: End-to-End Design and Implementation of Robust MPC on Resource-Limited Hardware Using Multi-Objective Bayesian Optimization and Deep Learning — ***Kimberly Chan***, *Joel Paulson, Ali Mesbah*

8:19 Paper 434b: On the Performance of Stochastic Predictive Control — ***Sungho Shin***, *Sen Na, Victor Zavala, Mihai Anitescu*

8:38 Paper 434c: Sparse-Identification-Based Predictive Control of Nonlinear Processes Using Noisy Process Data — ***Fahim Abdullah***, *Zhe Wu, Panagiotis Christofides*

8:57 Paper 434d: Partial Modifier Adaptation for Economic Optimization of Process Systems Under Frequent Disturbances and Structural Model Uncertainty — ***Gabriel Patron***, *Luis Ricardez-Sandoval*

9:16 Paper 434e: Machinelearning and Adaptive Model Predictive Control: Conflict or Conflux — *Zicheng Cai,* ***Erik Ydstie***

9:35 Paper 434f: Chromate Control in an Ion Exchange Process Under Uncertainty — ***Fred Ghanem***, *Kirti Yenkie*

9:54 Paper 434g: Parameter Estimation for Real-Time Optimization Under Model Uncertainty and Measurement Noise — ***Gabriel Patron***, *Luis Ricardez-Sandoval*

10:13 Paper 434h: Improving Computational Efficiency of Multi-Stage NMPC Using an Adaptive Horizon — ***Zawadi Mdoe***, *Dinesh Krishnamoorthy, Johannes Jäschke*

(435) Department Heads Forum (Invited Talks)

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, W-105A

Daniel Shantz, Chair
Clifford Henderson, Co-Chair
C. Heath Turner, Co-Chair

Sponsored by: Department Heads Forum

8:00: Welcome: Cliff Henderson, Dan Shantz, and Heath Turner

8:05: Salary Survey: Ty Johanes

8:35: ABET Update: Randy Lewis

8:45: NASEM Briefing on "New Directions for Chemical Engineering" (Speakers TBD)

9:15: State of the Institute: Darlene Schuster

9:45: Dean's Panel – Panelists TBD

10:25: Concluding Remarks

(436) Workshop: Roundtable Discussions on Current Topics in ChE Education

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, W-105C

Sandra Pettit, Chair
Jennifer Cole, Co-Chair

Sponsored by: Education

WELCOMING REMARKS

Poster 436a: Conference Highlights & Innovations — ***Jennifer Cole***

Poster 436b: Teaching and Assessing Teamwork — ***Matthew Cooper, Troy Vogel***

Poster 436c: Support for Mental Health — ***Sarah Wilson***

Poster 436d: Integrating the Arts, Humor, and Game-Based Theory — ***Peter Ludovice***

Poster 436e: Energy and Sustainability — ***J. Patrick Abulencia***

Poster 436f: Evidence-Based Instructional Practice - How to Convince the Skeptic — ***Margot Vigeant***

Poster 436g: Aiche's Ideal Path - Abet's Potential Role — ***Anthony Butterfield, Sindia M. Rivera-Jimenez***

PANEL DISCUSSION

(437) New Faculty Forum (Invited Talks)

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, W-105B

Burcu Beykal, Chair
Jerrod Henderson, Co-Chair

Sponsored by: Young Faculty Forum

8:00: Welcoming Remarks

8:05 Paper 437a: Becoming a Well-Rounded Scholar: A Spotlight on Effective Teaching & Mentoring — ***Allison Godwin***

8:35 Paper 437b: Staying True to Your Vision and Values As a Junior Faculty — ***Karthish Manthiram***

9:05: Discussion and networking

(438) Anisotropic Particles: Synthesis, Characterization, Modeling, Assembly, and Applications

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, N-232B

Isaac Torres Diaz, Chair
Bhuvnesh Bharti, Co-Chair

Sponsored by: Interfacial Phenomena

8:00 Paper 438a: Investigating How Entropy Compartmentalization Drives the Formation of Robust Host-Guest Structures — ***Tobias Dwyer***, *Timothy C. Moore, Joshua Anderson, Sharon Glotzer*

8:15 Paper 438b: Simulation Study of Colloidal Quasicrystals Engineered with DNA — ***Yein Lim***, *Sangmin Lee, Sharon C. Glotzer*

8:30 Paper 438c: Blade-Coating and Sintering of Mesomorphic Ceramics — *Xinquan Cheng, Wenshi Zhang, Shaw H. Chen,* ***Mitchell Anthamatten***

8:45 Paper 438d: Improved Characterization of Fluorescent Macromolecules Using Light Scattering — ***Zachariah Pittman***, *Christopher Kitchens*

9:00 Paper 438e: Synthesis and Characterization of Poly(amic-acid)-Silver Janus Nanoparticles for CO_2 Separation Applications — ***Matthew Webb***, *Michele Galizia, Sepideh Razavi*

9:15 Paper 438f: Computational Studies on the Structural Properties of Square Colloids with Offset Magnetic Dipoles — ***Matthew Dorsey***, *Orlin D. Velev, Carol Hall*

9:30 Paper 438g: Topological Interactions of Spiky Particles with a Planar Wall — ***Elizabeth Andrew***, *KaiLian Davis, Isaac Torres Diaz*

9:45 Paper 438h: Cloaking Anisotropic Capillary Interactions Using Nanoscale Surface Topography — *Samuel Trevenen,* ***Md Anisur Rahman***, *Heather S.C. Hamilton, Laura C. Bradley, Peter Beltramo*

10:00 Paper 438i: Order and Disorder in Inverse Opals — ***Jansie Smart***, *Kata Dorbic, Alessandro Parisotto, Marco Lattuada*

10:15 Paper 438j: Control of Phoretic Self-Propulsion through Particle Geometry: Slender-Body Analysis for an Asymmetric Bent Rod — *Arkava Ganguly,* ***Ankur Gupta***

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(439) Electrochemistry & Electrochemical Engineering for Environmental & Sustainability Applications

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, N-231A

Sneha Akhade, Chair
Won Tae Choi, Co-Chair

Sponsored by: Electrochemical Fundamentals

8:00: Break

8:20 Paper 439b: Modeling Pitting Corrosion in Petroleum Storage Tank — *Zaki Ahmed Choudhury,* ***Sidney Lin***, *Helen Lou*

8:40: Break

9:00 Paper 439d: Statistical and Energy Consumption Analyses of Multi-Factor Effect on Nutrient Removal and Recovery Via Electrochemical Animal Waste Remediation — ***Babatunde Ojoawo***, *Jason Trembly, Damilola Daramola*

9:15 Paper 439e: Energetic Benefits and Kinetic Drawbacks of Simultaneous Electrochemical CO_2 Capture Sorbent Regeneration and CO_2 Absorption — ***Jonathan Boualavong***, *Christopher Gorski*

9:30 Paper 439f: Insights into the Reaction Schemes of Furfural and 5-Hydroxymethylfurfural Reductions in Acidic Media over Copper — ***Andrew May***, *Seoyeong Lee, Sarvar Talipov, Elizabeth Biddinger*

9:45 Paper 439g: Electrocatalytic Oxidation of Methanol over Silver-Based Ag-M/C (M=Cu, Zn, Fe, Cr, Mn) Electrocatalysts Synthesized By Solution Combustion Technique — ***Khulood Logade***, *Sadiyah Shafath, Anand Kumar, Ibrahim Abu-Reesh*

10:00: Break

10:15 Paper 439i: Electrochemical K-Struvite Precipitation: Investigating the Role of pH and Water Chemistry — ***Amir Akbari***, *Lauren F. Greenlee*

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(440) Experimental Methods for the Study of Interfacial Phenomena

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, N-232C

Joseph Samaniuk, Chair

Sponsored by: Interfacial Phenomena

8:00 Paper 440a: Studying Fluid-Fluid Interfaces with a Custom Sub-Phase Exchange Microscopy Cell — *Benjamin Appleby, Arpit Mishra, David M. Goggin,* ***Joseph Samaniuk***

8:20 Paper 440b: Instrument for Measurement of Interfacial Structure-Property Relationships with Decoupled Interfacial Shear and Dilatational Flow: "*Quadrotrough*" — *Ying-Heng Tein, Benjamin Thompson, Charles F. Majkrzak, Brian Maranville, Damian Renggli, Jan Vermant,* ***Norman J. Wagner***

8:40 Paper 440c: Probing Adhesive Emulsions As a Function of Polymer and Surfactant Composition Via a Novel Microfluidic Platform — *Xiaotong Song, Emily Jamieson, Rico Tabor, Joe Berry,* ***Raymond Dagastine***

9:00 Paper 440d: Towards Constructing the Potential Landscape of a Colloidal Ellipsoid with Scattering Morphology Resolved Total Internal Reflection Microscopy (SMR-TIRM) — ***Jiarui Yan***, *Hairou Yu,* ***Christopher L. Wirth***

9:20 Paper 440e: A Two-Phase Model for Adsorption from Solution Using Quartz Crystal Microbalance with Dissipation — *Sarah Berlinger, Xunkai Chen, Maxim Yutkin,* ***Clayton Radke***

9:40 Paper 440f: Stratification in Micellar Foam Films As a Probe for Intermicellar Interactions — *Chrystian Ochoa, Shang Gao, Chenxian Xu, Samanvaya Srivastava,* ***Vivek Sharma***

10:00 Paper 440g: EDTA Modified Polyol Polymers for Performance Improvement of Laminating Adhesives — ***Xue (Ida) Chen***, *Yinzhong Guo*

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(441) Interfacial and Non-Newtonian Flows

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, N-232A

Hadi Mohammadigoushki, Co-Chair
Douglas Tree, Co-Chair

Sponsored by: Fluid Mechanics

8:00 Paper 441a: Combined Effect of Thinning and the Presence of Gas Boundary Layer on the Stability of a Thin Liquid Sheet — ***Soumya Kedia***, *Puja Agarwala, Mahesh Tirumkudulu*

8:15 Paper 441b: A Constitutive Model for Droplet Breakup in Unsteady Flows — ***Joseph Peterson***, *Vipin Michael, Ioannis Bagkeris*

8:30 Paper 441c: On the Critical Conditions of Thermoelastic Instabilities in Curvilinear Shear Flows: A Minimal Model — ***Radhakrishna Sureshkumar***, *Dennis Thomas, Bamin Khomami*

8:45 Paper 441d: Interfacial Instabilities during Displacement in Microchannels: The Effect of Boger Fluid in Channels with Bends — ***Seng Hoe (billy) Hue***, *Panagiota Angeli, Loic Chagot*

9:00 Paper 441e: A Novel Material for Oil-Spill Remediation That Is Both a Gel and an Absorbent — *Dan Walls, Emilie Espitalie, Anwu Li, Michael Gattrell,* ***John Frostad***

9:15 Paper 441f: Numerical Models and Experiments of Yield Stress Fluids Filling a Thin Mold. — ***Rekha Rao***, *Josh McConnell, Anne M. Grillet, Weston Ortiz*

9:30 Paper 441g: Impacts of Micellar Entanglement Density on Flows of Shear Banding Wormlike Micellar Fluids — *Peter Rassolov, Pamela Cook, Lin Zhou,* ***Hadi Mohammadigoushki***

9:45 Paper 441h: Instabilities of Dilute Wormlike Micelle Solutions in Circular and Planar Couette Flows — ***Richard Hommel***, *Michael Graham*

10:00 Paper 441i: Relation between Defect Dynamics and Rheology in a Sheared Lamellar Mesophase. — ***V Kumaran***

10:15 Paper 441j: Revisiting the Linear Stability of Surfactant Laden Liquid Film Flow inside of a Tube — ***Neha Jain***, *Gaurav Sharma*

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(442) Interfacial Processes at Biomembranes

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, N-231B

Peter Beltramo, Chair
Wade Zeno, Co-Chair

Sponsored by: Interfacial Phenomena

8:00 Paper 442a: *Interactions of Surfactants with the Bacterial Cell Wall and Inner Membrane: Revealing the Link between Aggregation and Antimicrobial Activity* — *Pradyumn Sharma, Srividya Parthasarathi, Rakesh Vaiwala, Nivedita Patil, Morris Waskar, Janhavi Raut, Jaydeep Basu,* ***Ganapathy Ayappa***

8:15 Paper 442b: Using Toxin-Membrane Interactions to Design an Antibiotic Delivery Vehicle — *Ziang Li,* ***Angela C. Brown***

8:30 Paper 442c: Antibody Binding As a Noninvasive Reporter of Cell Surface Heterogeneity and Organization — ***Daniel Arnold****, Yaxin Xu, Sho Takatori*

8:45 Paper 442d: Dynamic Interactions between Intrinsically Disordered Proteins and Curved Membrane Surfaces — ***Wade Zeno***

9:00 Paper 442e: Spindle-like Vesicle Shapes in External Fields — ***Rodrigo Reboucas****, Michael Miksis, Petia M. Vlahovska*

9:15 Paper 442f: Stability Analysis of Permeable Membrane Tubes Undergoing Osmotic Shocks — ***Ahmad Majed Alkadri****, Kranthi K. Mandadapu*

9:30 Paper 442g: Hydrophobicity and Functionality-Dependent Interactions of Poly- and Perfluoroalkyl Substances (PFAS) on Model Biological Membranes — ***Animesh Pan****, Jessica Alesio, Angela Slitt, Geoffrey D. Bothun*

9:45 Paper 442h: Permeability, Osmosis, and Hydrodynamics of Planar Lipid Membranes — ***Amaresh Sahu****, Alison Lui, Markita Landry, Kranthi K. Mandadapu*

10:00 Paper 442i: Triglycerides Stabilize Organic/Water Interfaces of Changing Area Via Conformational Flexibility — ***Thomas Kinard****, Steven P. Wrenn*

10:15 Paper 442j: Amphiphilic Proteins Coassemble into Multiphasic Condensates and Act As Biomolecular Surfactants — ***Fleurie Kelley****, Bruna Favetta, Roshan M Regy, Jeetain Mittal, Benjamin S. Schuster*

(443) Soft and Active Systems

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, N-231C

Sho Takatori, Co-Chair
Joseph Barakat, Co-Chair

Sponsored by: Fluid Mechanics

8:00 Paper 443a: Tunable Aggregation and Collective Hydrodynamics of Active Inclusions on Biological Membranes — ***Harishankar Manikantan***

8:15 Paper 443b: Topography-Driven Control of Active Filaments — ***Joseph Barakat****, Kevin Modica, Sho Takatori*

8:30 Paper 443c: Active Fluctuations Control Biopolymer Dynamics* — ***Ashesh Ghosh****, Andrew Spakowitz*

8:45: Break

9:00 Paper 443e: Out-of-Equilibrium Generic Modeling Predicts Isotropic-Nematic Emulsions with Diffuse Interfaces — ***Jonathan Salmeron-Hernandez****, Pablo Zubieta, Noe Atzin, Hans Christian Öttinger, Juan De Pablo*

9:15 Paper 443f: Rheotaxis of Active Droplet — *Prateek Dwivedi, Dipin Pillai,* ***Rahul Mangal***

9:30 Paper 443g: Wiggling of Motile Bacteria in Dilute, Low-Re Flows Near Walls — *Richard DeCurtis,* ***Sara Hashmi***

9:45 Paper 443h: Bacterial Swarm Simulations Highlight the Roles of Hydrodynamic Interactions, Cell Morphology and Steric Interactions on Emergent Patterns — ***Joshua Tamayo****, Arezoo Ardekani, Alison Patteson, Arvind Gopinath*

10:00 Paper 443i: Odd Transport in Active Matter — ***Cory Hargus****, Kranthi K. Mandadapu*

10:15 Paper 443j: Uphill Granular Heaping Flow Via Magnetically-Driven Particle Rotation — ***Samuel Wilson-Whitford****, Jinghui Gao, William Buckley, James Gilchrist*

(444) Thermophysical Properties and Phase Behavior I

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, N-222C

Erik Santiso, Chair
Sanket Deshmukh, Co-Chair
Hiroyuki Matsuda, Co-Chair
Harold Hatch, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

8:00 Paper 444a: Novel Mixed Matrix Polymer Membranes for Critical Gas Separations — ***Sanat K. Kumar***

8:40 Paper 444b: Surface Properties of Water Containing Mixtures Using Arpc-SAFT Equation of State — ***Fabian Brettschneider-Lazaro****, Sabine Enders*

9:00 Paper 444c: Combining Intermolecular Potentials for the Prediction of Fluid Phase Behavior — ***Richard Sadus***

9:20 Paper 444d: Thermodynamic Modeling of the Nature of Speciation and Phase Behavior of Binary and Ternary Mixtures of Formaldehyde, Water and Methanol — ***Malak Wehbe****, Andrew J. Haslam, Salvador Garcia Munoz, George Jackson, Amparo Galindo*

9:40 Paper 444e: Predicting the Phase Behavior of Highly Fluorinated Molecules Using the GC-SAFT-VR Equation of State — ***Alyssa Nelson****, Clare McCabe*

10:00 Paper 444f: Thermophysical Characterisation and Drop-in Assessment of Hydrofluoroethers in Organic Rankine Cycles — *Daniel Jovell, Rafael González-Olmos, Héctor Quinteros-Lama,* ***Felix Llovell***

(445) CO2 Industrial, Engineering and R&D Approaches

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, N-225B

Selen Cremaschi, Chair
Xiaonan Wang, Co-Chair

Sponsored by: Sustainability

8:00 Paper 445a: Techno-Economic Optimization of Electrochemical Reactors for CO_2 Reduction — *Lucas Cammann,* ***Isabell Bagemihl****, Maria Del Mar Pérez-Fortes, Volkert van Steijn, J Ruud Van Ommen*

8:18 Paper 445b: A Continuous, Integrated Electrochemical System for CO_2 Capture and Valorization — ***Rohan Sartape****, Aditya Prajapati, Meenesh Singh*

8:36 Paper 445c: Process Design and Optimization of Absorption-Based CO_2 Capture Processes with a Low-Pressure Flash Column — ***Haryn Park****, Joohwa Lee, Seokwon Yun, Jin-Kuk KIM*

8:54 Paper 445d: Design and Capability Requirements for a Direct Air Capture User Facility — ***Ronald Breault****, Justin Weber, Janice A. Steckel, Larry Kincell*

9:12: Break

9:30 Paper 445f: Multi-Objective Optimization of Carbon Capture Utilization and Storage Supply Chain — ***Manar Oqbi****, Dhabia Al-Mohannadi*

9:48 Paper 445g: Rate-Based Dynamic Modeling and Analysis of an Amine-Based Carbon Capture Unit for Flexible Operation — ***Paul Akula****, John C. Eslick,* ***Debangsu Bhattacharyya****, David Miller*

10:06 Paper 445h: Global Renewable Energy and Negative Emission Potential Observatory - in a Knowledge Graph Context — ***Lanyu Li****, Xiaonan Wang*

(446) Environmental Advance in Nuclear and Hazardous Waste Processing and Disposal

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, N-225A

Robert Peters, Chair
Reid Peterson, Co-Chair

Sponsored by: Solid and Hazardous Waste

8:00 Paper 446a: Visualization of 35+ Years of Data from the Doe Hanford Nuclear Reservation Site and the Associated Applications for Informing Key Tank Waste Treatment and Disposal Decisions — ***Courtney Bottenus***, *Heather B. Sabella, Erin L. McCann, Mark B. Triplett*

8:21 Paper 446b: Temperature Comparisons of Cesium Ion Exchange Performance with Crystalline Silicotitanate on Hanford Tank Waste — ***Amy Westesen***, *Emily Campbell, Sandra Fiskum, Truc Trang-Le, Ashley Williams, Andrew Carney, Reid Peterson, Matthew Landon, Kristin Colosi*

8:42 Paper 446c: Nitric-Glycolic Acid Flowsheet Implementation in the Defense Waste Processing Facility to Reduce Generation of Hydrogen — *Wesley Woodham,* ***Dan Lambert***, *Chris J. Martino, Bill Holtzscheiter, Terri Fellinger, Jeremiah Ledbetter, Dylan Baxter*

9:03 Paper 446d: Applicability of ATR-FTIR to Measure Dense Slurries: A Hanford Case Study — ***Rupanjali Prasad***, *Steven Crouse, Stefani Kocevska, Ronald Rousseau, Martha Grover*

9:24: Break

9:45 Paper 446f: Remediating Contaminated Land on Nuclear Sites — ***Prashant Mishra***, *Timothy N. Hunter, Jae Lee, David Harbottle*

10:06 Paper 446g: Integrated Approach for the Recovery of Metals and Valuable Materials from Waste Random Accesses Memory — ***Amrita Preetam***, *Satya Narayan Naik, K.K. Pant, Vivek Kumar*

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(447) Drug Delivery Strategies for Immunomodulation

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, N-126A

Jessica Larsen, Chair
Handan Acar, Co-Chair
Whitney Stoppel, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

8:00 Paper 447a: Delivery of Immunostimulatory Biologics for Skin Tissue Repair — ***Muhammad Raisul Abedin***, *Shubham Pallod, Jordan Yaron, Mallikarjun Gosangi, Jacquelyn Kilbourne, Kaushal Rege*

8:18 Paper 447b: Engineering a Logic-Gated Drug Delivery Platform for Cancer Immunotherapy — ***Blaise Kimmel***, *John Wilson*

8:36 Paper 447c: Localized Delivery of Tumor-Specific Antigen and Immune Checkpoint Antibodies to Induce Systemic Antitumor Immunity — ***Rong Tong***, *Eungyo Jang*

8:54 Paper 447d: Composite Deoxycholic Acid-Based Microparticles for Localized Adipose Tissue Reduction with Reduced Inflammation — ***Daniel Kupor***, *Michael L. Felder, Hanieh Safari, Omolola Eniola-Adefeso*

9:12 Paper 447e: Nanoparticle Delivery of Small Molecule Inhibitors to Treat Sting-Associated Inflammatory Diseases — ***Lucinda Pastora***, *Kyle Becker, Lihong Wang-Bishop, Plamen Christov, John Wilson*

9:30 Paper 447f: Optimized Lipid Nanoparticles and Delivery Conditions for State-of-the-Art Nebulized mRNA Delivery to the Lungs — ***Allen Jiang***, *Jacob Witten, Idris Raji, Sayo Eweje, Corina MacIsaac, Favour Oladimeji, Robert Langer, Daniel G. Anderson*

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(448) Fermentation and Process Engineering in Food and Bioprocess Industries

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, N-126B

Chang Dou, Chair
Maobing Tu, Co-Chair
Nuttha Thongchul, Co-Chair

Sponsored by: Food

8:00 Paper 448a: Relationship of Different Cultivation Conditions to the Efficacy of D-Lactic Acid Fermentation By *Sporolactobacillus Terrae*sbt-1 — *Nichakorn Amornbunchai,* ***Sitanan Thitiprasert***, *Nuttha Thongchul*

8:18 Paper 448b: Multi-Information Source / Objective Bayesian Optimization of Serum-Free Cell Culture Media for Cellular Agriculture — ***Zachary Cosenza***, *David E. Block*

8:36 Paper 448c: Fermentation Process Optimization for Enhancing D-Arabitol Production Performance in a Novel Strain of *Wickerharmomyces Anomalus* BKK11-4 — ***Nuttha Thongchul***, *Sitanan Thitiprasert, Jesnipit Tammakes*

8:54 Paper 448d: Exploring the Potential of NON-Growth Associated POLY-3-Hydroxybutyrate Production with Recombinant *Escherichia coli* through Dynamic Flux Balance Analysis — *Willians Santos,* ***Galo Carrillo le Roux***, *José Gregório Cabrera Gomez*

9:12 Paper 448e: Production of High-Value Methylxanthines Using Engineered Whole-Cell Biocatalysts — *Meredith Mock,* ***Ryan Summers***

9:30 Paper 448f: An Integrated Biological Process for the Valorization of Lignin-Derived Aromatics to Poly(4-vinylphenol) — *William Ederer,* ***Lakshmi Meghana Bathineni***, ***Apurv Mhatre***, *Hemant Choudhary, John M. Gladden, Alberto Rodriguez, Arul Mozhy Varman*

9:48 Paper 448g: [Keynote] Enhancing Prehydrolysates Fermentability By Adding Nucleophilic Amino Acids and Proteins in Biomass Pretreatment — *Yequan Sheng, Yu Zhang,* ***Maobing Tu***

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(449) New tools & strategies for metabolic engineering

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, N-125A

Nathan Crook, Chair
Han Li, Co-Chair

Sponsored by: Bioengineering

8:00 Paper 449a: Redox Balance-Based Growth Selection As a Universal Tool for Enzyme Engineering — ***Han Li***

8:18 Paper 449b: Utilizing Antimicrobial Peptide for Regulation of Global Metabolism and Its Application in Microbial Biosynthesis — ***Lei Zhuang***, *Yuxin Liu, Haoran Zhang*

8:36 Paper 449c: Cascaded Dynamic Regulation for Attenuated Metabolic Imbalance and Increased Naringenin Production — ***Tian Jiang***, *Chenyi Li, Yusong Zou, Jianli Zhang, Qi Gan, Yajun Yan*

8:54 Paper 449d: Dynamic Regulation of Metabolic Pathways with Toehold-Gated dCas9 Regulators — ***Alexander Perl***, *Manish Rai, Hunter Dalton, Richa Nathan, Mattheos Koffas, Wilfred Chen*

9:12 Paper 449e: MULTI-Sculpt – Multiplex Integration Via Selective, CRISPR-Mediated, Ultra Long Pathway Transformation in Yeast for Natural Product Synthesis — ***Franklin Gong***, *Jianing Han, Sijin Li*

9:30 Paper 449f: Improving Transformation Efficiencies in *Synechococcus* Sp. Via the Novel Combination of DNA Methylation and Plasmid Multimers — ***Cody Kamoku***, *Christopher Jones, David Nielsen*

9:48 Paper 449g: Teaching an Old Dog New Tricks — Elucidating Core Design Principles to Engineer Yeasts As Microbial Factories and Disease Models — ***Zengyi Shao***, *Deon Ploessl, Yuxin Zhao*

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(450) Synthetic biology of underutilized organisms with unique phenotypes

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, N-125B

Benjamin Woolston, Chair
Jason Boock, Co-Chair

Sponsored by: Bioengineering

8:00 Paper 450a: Synthetic Biology Tool Development Advances Predictable Gene Expression in the Metabolically Versatile Soil Bacterium *Rhodopseudomonas Palustris* — ***Mark Kathol***, *Cheryl Immethun, Taity Changa, Rajib Saha*

8:18 Paper 450b: Enhanced Synthetic Biochemistry Systems Enabled By Improvements in *Bacillus subtilis* Spore-Display — ***Trevor Nicks***, *Todd C. Chappell, Vikas D. Trivedi, Karishma Mohan, Nikhil Nair*

8:36 Paper 450c: A Modular Synthetic Biology Toolkit for Environmental Actinobacteria — *Zachary Jansen, Matan Lieber-Kotz,* ***Ross Thyer***

8:54 Paper 450d: Development of a Synthetic Biology Toolbox for Soil Bacteria — ***Maya Venkataraman***, *Taylor Cook, Brian F. Pfleger*

9:12: Break

9:30 Paper 450f: High Efficiency Multiplexed Cytosine Base Editing in Yarrowia Lipolytica — ***Vijaydev Ganesan***, *Dheeraj Pedada, Anthony Stohr, Jaya Gupta, Mark Blenner*

9:48 Paper 450g: Onboarding Environmental Microbes for Efficient (re)Use of Renewable Feedstocks and Consumer Wastes in Biomanufacturing — ***Kevin Solomon***

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(451) Advanced Biomass Conversion Technologies

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, N-228B

Xinshu Zhuang, Chair
Shijie Liu, Co-Chair

Sponsored by: Forest and Plant Bioproducts Division

8:00 Paper 451a: Low Temperature Hydrothermal Liquefaction of a Mixture of Lignin and Hemicellulose Derived Product Mixture — ***Sampath Gunukula***, *Sampath Karunarathne, Clayton Wheeler*

8:25 Paper 451b: Microwave Heated Pretreatment of Agricultural Residues with Deep Eutectic Solvents to Isolate Lignin-Carbohydrate Complex for Renewable Fuel and Material Applications — ***Sanphawat Phromphithak***, ***Thossaporn Onsree***, *Jochen Lauterbach, Nakorn Tippayawong*

8:50 Paper 451c: Improving Bamboo's Fuel and Storage Properties with a Net Energy Export through Torrefaction Paired with Catalytic Oxidation — ***Nepu Saha***, *Eric Fillerup, Brad Thomas, Corey Pilgrim, Thomas Causer, Dan Herren, Jordan Klinger*

9:15 Paper 451d: Computational Fluid Dynamic Simulations for Woodchips Chemical Looping Gasification in a Bubbling Fluidized Bed Fuel Reactor — ***Hessamedin Naeimi***, *Afsaneh Khajeh, Lijun Wang, Abolghasem Shahbazi*

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(452) Biomass Characterization, Pretreatment, and Fractionation

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, N-228A

Bandaru V. Ramarao, Chair
Shijie Liu, Co-Chair

Sponsored by: Forest and Plant Bioproducts Division

8:00 Paper 452a: Using Artificial Neural Networks to Estimate Xylose Conversion and Furfural Yields in Autocatalytic, Organic/Aqueous Solvent Systems — *Adam L. Job, Sarah Stratton, Charles E. Umhey, Karlene A. Hoo,* ***Stephanie Wettstein***

8:15 Paper 452b: Valorization of Bioenergy Crops for Recovery of Anthocyanins and Sugars — ***Shivali Banerjee***, *Erik Sacks, Vijay Singh*

8:30 Paper 452c: Effect of Fines % on Ultrasonic Dewatering of Cellulose Nanofibrils — ***Udita Ringania***, *Robert Moon, M. Saad Bhamla*

8:45 Paper 452d: Characterization of Brewer's Spent Grain through Thermogravimetric Analysis for Energy Production — ***Spencer Fogelquist***, *David Wagner*

9:00 Paper 452e: High-Grade Lignin Production: Evolution of Lignin Structure through γ-Valerolactone-Assisted Hydrolysis of Biomass — *Feng Cheng, Sarah Liu, Steven Karlen, Hoon Kim, Fachuang Lu, John Ralph, George Huber, James A. Dumesic,* ***Leoncio Santiago Martínez***

9:15 Paper 452f: Enhanced Feedstock Characterization and Modeling to Facilitate Optimal Preprocessing and Deconstruction of Corn Stover — *Dylan Cousins, William Otto, Asif Hasan Rony, John E. Aston,* ***David Hodge***

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(453) Value-Added Chemicals from Natural Gas II

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, W-103A

Dushyant Shekhawat, Chair
Goetz Veser, Co-Chair
Jianli Hu, Co-Chair

Sponsored by: Fuels and Petrochemicals Division

8:00 Paper 453a: Direct Methane Conversion By Atomically Thin Platinum Nanolayers on Two Dimensional Metal Carbides — ***Yue Wu***

8:19 Paper 453b: Oxidative Coupling of Methane Catalysts: Developing Structure-Property Relationships for High-Performance Metal Oxide Systems — ***Mariano D. Susman***, *Matteo Ferri, Raffaele Cheula, Hien N. Pham, Abhaya K. Datye, Sivadinarayana Chinta, David West, Matteo Maestri, Jeffrey Rimer*

8:38 Paper 453c: Pt-Based Monolithic Catalysts for Oxidative Coupling of Methane: Effect of Catalyst Formulation and Operation Parameters — ***Sven Schardt***, *Ahmet Celik, Jaspreet Chawla, Simon Bastian, Stephan A. Schunk, Patrick Lott, Olaf Deutschmann*

8:57 Paper 453d: New Insights into the Effect of CO2 on Oxidative Coupling of Methane (OCM) — ***Yonggang Cheng***, *Pedro Mendes, Joris Thybaut*

9:16 Paper 453e: Non-Catalytic Direct Partial Oxidation of Methane to Methanol in a Microreactor — ***Kelly Cohen***, *Justin Blanchard, James Dorman, Kerry Dooley*

9:35 Paper 453f: Electrochemical Oxidation of Methane to Methanol on Electrodeposited Transition Metal Oxides Under Ambient Temperature — ***Kangze Shen***, *Yu-Chao Huang, Joonbaek Jang, Carlos Morales-Guio*

9:54 Paper 453g: Ethane Dehydrogenation Using Liquid Metal Catalysts — ***Aime Laurent Twizerimana***, *Kaylen Ocampo, Aaditya Hari Bharanidharan, Kayle McGaughy, Mohammad S. Masnadi, Goetz Veser*

10:13 Paper 453h: Ethane Oxidative Dehydrogenation By CO_2 over Stable Csru/CeO_2 Catalyst — ***Xiaoyan Wang***, *Yuxin Wang, Brandon Robinson, Jianli Hu*

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(454) Conversion of plastic wastes to high value products

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, N-230

Zheng Liu, Chair
Hsi-Wu Wong, Co-Chair

Sponsored by: Green Process and Product Engineering

8:00 Paper 454a: Upcycling Polyolefin Waste into Performance Elastomers — ***Weizhong Zou***, *Alexis Hocken, Bradley Olsen*

8:30: Break

9:00 Paper 454c: First-Principles Kinetic Modeling System for the Pyrolysis of Waste Plastics — ***Pratyush Agarwal***, *David Tremblay, Zhen Hou, Shu Wang*

9:30 Paper 454d: Kinetics Insights of Waste Plastic Pyrolysis with Auto-Fragment Modeling (AFM) — ***Yen-Ting Wang***, *Matthew Prendergast, William Green*

10:00 Paper 454e: Solvolysis Liquefaction of Low-Rank Coals and Polyolefin Waste-Plastics-Derived Liquid into Mesophase Pitch Intermediates to Manufacture Value-Added Carbon Materials — ***Wenjia Wang***, *Karissa Jolley, Mitchell G Nelson, Eric Eddings*

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(455) Process Intensification and Modular Manufacturing: Intensified Reaction and Separation Processes

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, N-221B

Ignasi Palou Rivera, Chair
Patricia Gillenwater, Co-Chair

Sponsored by: Process Intensification & Modular Chemical Processing

8:00 Paper 455a: A Low-Temperature Hollow Fiber Membrane Reactor for Intensified Propane Dehydrogenation — ***Lu Liu***, *Antara Bhowmick, Dongxia Liu, Chen Zhang*

8:20 Paper 455b: Experimental Optimization of Process Parameters for Ammonia Separation to Achieve +95% Ammonia Stream — ***Fouzia Hasan Nowrin***

8:40 Paper 455c: Intensification of Dispersants Production Via Thin Film Evaporation for Simultaneous Reaction and Separation — ***Riddhesh Patel***, *Nasser Al Azri, Hari Mantripragada, Glenn Cormack, Nicolas Proust, Robert M. Enick, Goetz Veser*

9:00 Paper 455d: Thermodynamically Tuned Redox Catalyst for Ethane to Liquid Fuels Via Chemical Looping in Simple, Distributed Reactors — ***Luke Neal***, *Leo Brody, Fanxing Li*

9:20 Paper 455e: Techno-Economic Analysis of Ultrasound Technology for Ethanol-Water Mixture Separation Process — ***Jiwoo Ha***, *Hyerin Seo, Junli Liu, Hao Feng, Nikolaos Sahinidis, Jonggeol Na*

9:40 Paper 455f: Integrated Direct Carbon Capture and Oxidative Dehydrogenation of Ethane with CO_2 at Isothermal Conditions over Dual-Functional Adsorbent/Catalyst Composite Monoliths — ***Khaled Baamran***, *Shane Lawson, Ali Rownaghi, Fateme Rezaei*

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(456) Division Plenary: Materials Engineering & Sciences Division (Invited Talks)

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, N-129AB

Julie Champion, Chair
Bradley Olsen, Co-Chair
April Kloxin, Co-Chair

Sponsored by: Materials Engineering and Sciences Division

8:00 Paper 456a: Braskem Award Lecture: Engineering the Crystallization and Semicrystalline State of Polymers through Molecular Modeling — ***Gregory Rutledge***

8:30 Paper 456b: Owens Corning Early Career Award Lecture: Organic Semiconductor-Incorporated Perovskites (OSiP) – a New Family of Hybrid Electronic Materials — ***Letian Dou***

9:00 Paper 456c: Engineering Protein-Based Materials with Modular Functionalities — ***Wilfred Chen***

9:30 Paper 456d: Challenges and Opportunities in the Development of Advanced Battery Materials — ***Perla Balbuena***

10:00 Paper 456e: Design and Scalable Fabrication of Three-Dimensional Hierarchically Porous Superstructures— for Flexible Self-Powered Electronics, Catalysis, and Water Purification — ***Donglei Fan***

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(457) Area Plenary: Bionanotechnology (Invited Talks)

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, W-104A

Lorraine Leon, Chair
Catherine Fromen, Co-Chair
Elizabeth Nance, Co-Chair

Sponsored by: Bionanotechnology

8:00 Paper 457a: Molecular Engineering of Biomimetic Condensates and Polyelectrolyte Complex Micelles — ***Lorraine Leon***

8:50 Paper 457b: Disease in a Dish: Engineering Tissue Environment to Recreate Snapshots of Disease Progression — ***Srivatsan Kidambi***

9:40 Paper 457c: Design of Targeted Antimicrobial Macromolecules — ***Christopher Alabi***

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(458) Nanoscale Science and Engineering Forum I (All Papers)

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, W-104B

Yoonjee Park, Chair
Yeongseon Jang, Co-Chair

Sponsored by: Nanoscale Science and Engineering Forum

8:00 Paper 458a: Light-Induced Chiral Metamaterial Printing — ***Ji-Young Kim***, *Connor McGlothin, Minjeong Cha, Emine Sumeyra Turali-Emre, Wonjin Choi, Nicholas Kotov*

8:19 Paper 458b: Effect of Pd Precursor Salt Type and Temperature on Synthesizing Five-Fold Pentagonal Pd Nanorods Using L-Ascorbic Acid in Segmented Millifluidic Flow Reactors (SMFRs) — ***Chamath Vindula Basnayake Pussepitiyalage***, *Shohreh Hemmati*

8:38 Paper 458c: Controlled Polymer Nanoparticle Synthesis Using a Jet Mixing Reactor — ***Faiz Khan***, *Xiangming Gu, Jiaqi Luo, Nicholas Brunelli, Barbara E. Wyslouzil, Jessica Winter*

8:57 Paper 458d: Continuous Millifluidic Synthesis of One-Dimensional Silver Nanostructures Using Tannic Acid As Reducing and Capping Agent: Parametric Study and Kinetic Behavior — ***Sina Kaabipour***, *Shohreh Hemmati*

9:16 Paper 458e: Sonochemical Method for High-Throughput Synthesis of Inorganic Nanostructures — ***Fabio Baum***, *Maria Politi, Cameron Tavakoli, Josiah S. Mace, Kiran Vaddi, Joshua Vasquez, Nadya Peek, Lilo Pozzo*

9:35 Paper 458f: Extending the Diatom's Color Palette: Bio-Inspired, Colloid-Templated Structures for Vivid Coloration and Optical Sensing — ***Pavel Shapturenka***, *Isaac Zakaria, Helen Stute, Fabian Birkholz, Michael Gordon*

9:54 Paper 458g: Magnetically Aligned Metal-Organic Deposition (MOD) Ink Based Functional Surfaces with Enhanced Wettability — ***Seyed Alireza Rozati***, *Anju Gupta*

10:13 Paper 458h: Assembly of Photoluminescent Silicon Nanocrystals with Reversible Covalent Bonds — ***Benjamin Stacy***, *Brian A. Korgel*

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(459) Mixing Scale-Up and Scale-Down Issues in Pharmaceutical Processes

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, N-227C

Luis Sierra, Chair
Chadakarn Sirasitthichoke, Co-Chair

Sponsored by: North American Mixing Forum

8:00: Break

8:30 Paper 459b: Using CFD to Predict Mixing Coefficients for Scale up — ***Darren Cappelli***

9:00 Paper 459c: A Design of Experiment (DOE)-Based Approach for Bioreactor Scale up and Cell Metabolic Reactions — *Sravan Nallamothu,* ***Hossam Metwally***, *Sivasubramani Krishnaswamy, Sophie Collin, Clementine Shao, Marc Horner*

9:30 Paper 459d: Scale-Down of Viral Inactivation Step: Principles and Practical Challenges — ***Zbynek Kalal***

10:00 Paper 459e: Application of Gas-Liquid Mass Transfer Coefficient Fitting Techniques in Batch Reactors for Scale-up — ***Kira Ragazzo***, *Jeffrey A. Nye, Shulin Wu, Xiaowen Zhao, Candice Joe, Megan Emmanuel, Antonio C. Ferretti, Richard Heid*

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(460) Crystallization in Process Development

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, W-106A

Bruce Hook, Chair
Moo Sun Hong, Co-Chair

Sponsored by: Solids Flow, Handling and Processing

8:25 Paper 460b: Enhancement of Crystallization Behavior for Solid Solution Separation Using Different Antisolvents — ***Vico Tenberg***, *Masoud Sadeghi, Andreas Seidel-Morgenstern, Heike Lorenz*

8:50 Paper 460c: Effect of Low Level Organic Impurities on Pharmaceutical Crystallization Kinetics and Impact on Physical Properties — ***Saurin Hiren Rawal***, *Jeremy Merritt*

9:15: Break

9:40 Paper 460e: Shaping Particle Size Distribution of a Metastable Polymorph in Additive-Assisted Reactive Crystallization By the Taguchi Method — ***Hung Lin Lee***, *Chia Ling Yang, Tu Lee*

10:05 Paper 460f: Continuous Crystallization in Slug Flow Aided with Indirect Focused Ultrasonication — ***Sunuk Kim***, *Consuelo Del Pilar Vega-Zambrano, Mingyao Mou, Frank Gupton, Mo Jiang*

(461) Particle Agglomeration and Granulation Processes

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, W-106C

Brendon Ricart, Chair
Shankali Pradhan, Co-Chair

Sponsored by: Particle Production and Characterization

8:00 Paper 461a: Influence of Impeller Geometry on the Formation of Spherical Agglomerates — ***Victoria Kitching***, *Kate Pitt, Bilal Ahmed, James D. Litster, Rachel M. Smith*

8:15 Paper 461b: Novel Approach for the Characterization of Powder Caking — ***Alessandra Hausmann***, *Britta Buck, Laura Shaw, Tom Simons, Daryl Williams*

8:30 Paper 461c: Granulation of Reactive Pyrotechnic Composition for Temperature Mapping of Coal-Boilers — ***Swarom Kanitkar***, *Biswanath Dutta, Daniel Haynes, Edward Sabolsky, Benajmin Chorpening*

8:45 Paper 461d: Sequential Fixed Fluidized Bed Foam Granulation (SFFBFG) and Drying: Multivariate Model Development for Water Content Monitoring with Near-Infrared Spectroscopy — *Abdoulah Ly, Ryan Gosselin, Esma Ines Achouri,* ***Nicolas Abatzoglou***

9:00 Paper 461e: A Combined Numerical Modelling and Laboratory Investigation into the Relationship between the Power to Mass Ratio, Turbulent Eddy Dissipation and Particle Size Distribution — *Justin O'Sullivan,* ***Kate O'Dwyer***

(462) Particle Technology: Honoring John Carson

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, W-106B

Karl Jacob, Chair

Sponsored by: Solids Flow, Handling and Processing

8:00 Paper 462a: Opening Remarks and Comments on John Carson — ***Karl Jacob***

8:10 Paper 462b: Industrial Needs in Solids Handling — ***Tim Bell***, *Massih Pasha*

8:35 Paper 462c: Thirty Years Along a Particle Technology Pioneer — ***Herman Purutyan***

9:00 Paper 462d: Irregular Soil Particle Shape Modeling — ***Jennifer Curtis***

9:25 Paper 462e: Innovation Challenges in Solids Processing at Industrial Scales — ***Shrikant Dhodapkar***

9:50 Paper 462f: Reflections on My Career in Particle Technology — ***John Carson***

(463) Plenary Session: Pharmaceutical Discovery, Development and Manufacturing Forum (Invited Talks)

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, N-124AB

Andreas Bommarius, Chair
Kevin D. Seibert, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

8:00 Paper 463a: mRNA Therapeutics – New Insights into the Sterile Filtration Process — ***Andrew Zydney***

8:50 Paper 463b: Process Innovation in Oligonucleotide Manufacturing — ***Firoz Antia***

9:40 Paper 463c: Innovating for the Big Challenges — ***Celia Cruz***

(464) Materials and Processes for Water Purification and Desalination I

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, N-222A

Sitaraman Krishnan, Chair

Sponsored by: Product Design

8:00 Paper 464a: Advancing Separation Processes and Water Purification Techniques Using Carbon Nanomaterial-Based Aerogels — *Darren Smith, Badri Hamwi,* ***Reginald Rogers Jr.***

8:25 Paper 464b: Graphene-Mediated Removal of Microcystin-LR for Treatment of Harmful Algal Blooms — ***Jesse Roberts***, *Chris Griggs, Luke A. Gurtowski, Kristina Johnson, Sarah Grace Zetterholm, Angela Evans, Sheila Mcleod, Justin Puhnaty*

8:50 Paper 464c: Electrospun Carbon/Iron Composite Fibers and Their Utilization As Adsorbents for Enhanced Cr(VI) Removal from Water — *Yang Lu, Hadi Rouhi, Colton Duprey, Elham Ghalavand,* ***Evan Wujcik***

9:15 Paper 464d: Neutron Characterization of Aluminum Electrodes Used in Electrocoagulation Pretreatment of Groundwater for Silica and Hardness Removal — ***Gyoung Gug Jang***, *Yousuf Bootwala, Alexander Wiechert, Marta Hatzell, Sotira Yiacoumi, Yuxuan Zhang, Candice Halbert, Jong K. Keum, David Jassby,* ***Costas Tsouris***

9:40 Paper 464e: Adsorptive Removal of Polystyrene Nanoplastics from Water Using MIL-101(Cr) Metal Organic Framework — ***Sweta Modak***, *Medha Kasula, Milad Esfahani*

10:05 Paper 464f: Effect of Thermochemical Process Parameters on Adsorption of Microcystin-LR and Nutrients on Biomass-Derived Pyrolyzed Hydrochar — ***Cadianne Chambers***, *Md Arafat Ali, Nirupam Aich, Sumit Sharma, Toufiq Reza*

(465) Adsorbent Materials: MOFs

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, N-131C

Armin Ebner, Chair
Krista Walton, Co-Chair

Sponsored by: Adsorption and Ion Exchange

8:00 Paper 465a: Metal-Organic Frameworks As Suitable Candidates for Atmospheric Water Harvesting — ***Saumil Chheda***, *Nikita Hanikel, Xiaokun Pei, Hao Lyu, WooSeok Jeong, Joachim Sauer, Omar Yaghi, Joern Siepmann, Laura Gagliardi*

8:18 Paper 465b: Deducing Information about Defects in MOFs Using Their Water Stability — ***Shubham Jamdade***, *Salah Eddine Boulfelfel, Hanjun Fang, David Sholl*

8:36 Paper 465c: Formulation and Processing of Magnetic-MOF Composite Structured Monoliths for Light Olefin/Paraffin Separation — ***Khaled Baamran***, *Ali Rownaghi, Fateme Rezaei*

8:54 Paper 465d: Carbon Dioxide Capacity Retention on Elastic Layered Metal Organic Frameworks Subjected to Hydrothermal Cycling — ***Christian Lastoskie***

9:12 Paper 465e: Trivalent metals on MOFs for SO2 adsorption — ***Chengzhai Wang***, *Krista Walton*

9:30 Paper 465f: Investigation of the Properties of MOFs for Adsorption of PFOS: Comparative Study of MIL 101 (Cr), MIL 101 (Cr)-AC, MIL 101 (Cr)-NH_2 , & MIL-53(Al) BPDC with Activated Carbon — ***Jasneet Pala***, *Tin Le, Medha Kasula, Milad Esfahani*

9:48 Paper 465g: Understanding Small Molecule Binding Potential Landscapes Near Open-Metal Sites in M-MOF-74 (M=Mg, Mn, Ni, Zn) — ***Ishan Pandey***, *Chau-Chyun Chen, Joshua Howe*

10:06 Paper 465h: Effect of Topology and Structural Tunability on Selective Capture of CO_2 Using Zeolitic Imidazolate Frameworks — ***Rimita Bose***, *Parasuraman Selvam, Niket Kaisare*

(466) Developments in Extractive Separations: Solvents

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, N-132A

David Cantu, Chair
George S. Goff, Co-Chair

Sponsored by: Extractions

8:00 Paper 466a: Light-Responsive Azobenzocrown Ethers for Enhanced Cs^+ Extraction from Contaminated Aqueous Sources — ***John Edward Sio***, *Erwin Escobar, Khino Parohinog, Wook-Jin Chung, Grace Nisola*

8:20 Paper 466c: Boron Extraction from Aqueous Medium Using a Designed Deep Eutectic Solvent and the Regeneration of the Used Solvent — *Aya Ghazal, Hadil Abu Khalifeh,* ***Ioannis Zuburtikudis****, Inas AlNashef*

8:40 Paper 466d: Molecular Design of Solvents for Temperature Swing Solvent Extraction — ***Lauren Ward****, Luke Rakers, Shuai Qian, Gabriel Barbosa, C. Heath Turner, Jason Bara,* ***Steven Weinman***

9:00 Paper 466e: Relative Stability Complexes of Lanthanide-Ligand Complexes from Computation — ***Ravi O'Brien****, Thomas Summers, Danil Kaliakin, David Cantu*

9:20 Paper 466f: DFT Calculations for Solvent Extraction Desalination: Electrostatic Potential, Hydrogen Bonding, and Solvation Free Energy — ***Xiaoyang Liu****, C. Heath Turner*

9:40 Paper 466g: COSMO Screening of Hydrophobic Deep Eutectic Solvents for Platform Chemical Extraction from Water — ***Thomas Quaid****, Toufiq Reza*

(467) Next Generation Biomolecules and Bioprocesses

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, N-130

Ketki Behere, Chair
Piran Kidambi, Co-Chair

Sponsored by: Bio Separations

8:00 Paper 467a: Lanthanide Binding Tag Peptides for the Foam Fractionation of Rare Earth Elements — ***Luis Ortuno****, Pan Sun, Stephen Crane, Dr. Kathleen J. Stebe, Wei Bu, Binhua Lin, Mark Schlossman, Raymond S. Tu, Charles Maldarelli*

8:20 Paper 467b: Eco-Friendly Detergent Combo for Viral Inactivation in Protein Manufacturing — ***Yuanyuan Ji****, Melissa Holstein, Zhi Li, Dong Yang, Sanchayita Ghose*

8:40 Paper 467c: Magnetic Fractionation of Red Blood Cells Based on Oxygen Saturation in Sickle Cell Disease. — ***Jacob Strayer****, Mitchell Weigand, Xian Wu, Hyeon Choe, Jeffrey Chalmers*

9:00 Paper 467d: Ribosomal Peptides Containing Fatty Acyl Moieties Synthesized By Noncannonical Kas III Enzymes — ***Hengqian Ren****, Chunshuai Huang, Haiyang Cui, Yuwei Pan, Huimin Zhao*

9:20 Paper 467e: The Surface Rheology of Interacting Peptide Surfactants and Rare Earth Elements at Air-Water Interfaces — ***Stephen Crane****, Jiayi Deng, Mehdi Molaei, Luis Ortuno Macias, Dr. Kathleen J. Stebe*

9:40 Paper 467f: Understanding Cerium Binding Affinity in Lanmodulin Derived Peptides — ***Geeta Verma****, Jacob Hostert, Julie N. Renner*

10:00 Paper 467g: Monolithic Silica Microchannels Enable Thin Layer Chromatography Analysis of Single Cells — *Yuli Wang,* ***Ming Yao****, Christopher Sims, Nancy Allbritton*

(468) Nucleation and Growth II

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, N-131A

Gaurav Giri, Chair
Mohammad Azad, Co-Chair

Sponsored by: Crystallization and Evaporation

8:00: Introductory Remarks

8:03 Paper 468a: Two-Step Nucleation Mechanism Drives Crystal Structure Formation By Selective Desolvation — *Anish Dighe,* ***Prem Podupu****, Paria Coliaie, Meenesh Singh*

8:32 Paper 468b: *In-Silico* Molecular Simulation Methods for Crystal Nucleation in Solution — ***E. Daniel Cárdenas-Vásquez****, James Savino, Erik Santiso*

9:01 Paper 468c: Selective Construction of $CaCO_3$ Superstructures *Via* Homoporous Interfacial Crystallizer — ***Xiaobin Jiang****, Mengyuan Wu,* ***Gaohong He***

9:30 Paper 468d: Application of Molecular Theory to Understand the Mechanism of NaCl Crystal Nucleation from Aqueous Solution — ***Ravi Kumar Reddy Addula****, Aravind Unni, Sudeep Punnathanam*

9:59 Paper 468e: Bimodal Impacts of Modifiers on Nucleation and Growth: Case of Calcium Oxalate Monohydrate — ***Bryan Alamani****, Rica Jan Ondoy*

10:28: Concluding Remarks

(469) Water Treatment, Desalination, and Reuse II

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, N-131B

Alexander Lopez, Chair
Lucy Mar Camacho, Co-Chair

Sponsored by: Membrane-Based Separations

8:00 Paper 469a: Process Modeling of Intermittent Wellhead RO Water Treatment Operation Via Integration of Self-Organizing Maps and Long Short-Term Memory Recurrent Neural Network (RNN) — ***Yang Zhou****, Nora Marki, Bilal Khan, Yoram Cohen*

8:21 Paper 469b: A Study of a Multi-Step Membrane-Based Desalination Process for Resource Recovery — ***Hossein Dallalzadeh Atoufi****, David Lampert*

8:42 Paper 469c: Recovery of Organics from Humidification-Dehumidification of Hydraulic Fracturing Wastewater Using Deep Eutectic Solvents — ***Elnaz Nikooei****, Iolar Lima, Bahman Abbasi, Nick AuYeung*

9:03 Paper 469d: Multilayered MFI-Zeolite Nanosheet Plates for Tiling Membranes on Porous Polyvinylidene Fluoride Substrates for Wastewater Desalination — ***Zishu Cao****, Landysh Iskhakova, Xinhui Sun, Zhong Tang, Junhang Dong*

9:24 Paper 469e: RO Membrane Characterization and Modeling Under High Pressure — ***Jeffrey McCutcheon****, Mi Zhang, Yara Suleiman, Danh Nguyen, Sina Shahbazmohamadi, Vimal Ramanuj, Ramanan Sankaran, Ying Li*

9:45 Paper 469f: Ultra-Strong Polymeric Hollow Fiber Membranes for Saline Dewatering and Desalination — ***Can-Zeng Liang****, Mohammad Askari, Looh Tchuin (Simon) Choong, Tai-Shung Chung*

10:06 Paper 469g: Electrospun Liquid-Infused Membranes for Emulsified Oil/Water Separation — ***Chen Song****, Gregory Rutledge*

(471) Tissue Engineering, Bioprinting, and Regenerative Medicine

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, N-126C

Jamie Spangler, Chair
Shachi Mittal, Co-Chair

Sponsored by: Chemical Engineers in Medicine

8:00 Paper 471a: Mitochondrial Mechanisms Underlying NANOG Induced Reversal of Aging — ***Debanik Choudhury****, Na Rong, Nika Rajabian, Georgios Tseropoulos, Pihu Mehrotra, Ramkumar Thiyagarajan, Pedro Lei, Izuagie Ikhapoh, Kenneth Seldeen, Bruce Troen, Stelios Andreadis*

8:22 Paper 471b: Effects of Processing Conditions on the Macroscopic Properties of Cellulose Filled Hydrogel Scaffolds Using UV Rheology — ***Bobby Haney***, *Subramanian Ramakrishnan*

8:44 Paper 471c: 3D Bioprinting of iPSC Derived Islet Organoids in Hydrogel Constructs — ***Miranda Poklar***, *Ben Mizerak, Ravi Krishnamurthy, Connor Wiegand, Prashant Kumta, Ipsita Banerjee*

9:06 Paper 471d: Engineering the Skeletal Muscle for Improved Innervation after Peripheral Nerve Injury — ***Pihu Mehrotra***, *Shahryar Shahini, Nika Rajabian, Yali Zhang, Jianmin Wang, Song Liu, James Jablonski, Susan Udin, Stelios Andreadis, Kirkwood Personius*

9:28 Paper 471e: Regeneration of the Epithelium Layer Using Fibrous Biomimetic Basement Membranes in a Mouse Dermal Wound Model — ***Dina Gadalla***, *Maeve Kennedy, David Lott*

9:50 Paper 471f: Photochemical Reaction Kinetics and Thermodynamics of Light-Induced Collagen Cross-Linking with Rose Bengal for Suture-Less Wound and Incision Closure and Repair — ***Alan Aguirre-Soto***

(472) Next-Gen Manufacturing in Chemical and Energy Systems

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, N-221A

Alexander Dowling, Chair
Kirti Yenkie, Co-Chair

Sponsored by: Next-Gen Manufacturing

8:00 Paper 472a: Keynote Talk-Self-Driving Fluidic Micro-Processors for Accelerated Discovery and Manufacturing of Energy Materials — ***Milad Abolhasani***

8:30 Paper 472b: Keynote Talk-Advancements in Manufacturing Via Strategic Assemblies of Bio-Based Polymers and Composites and Adaptive 3D Printing Techniques — ***Joseph Stanzione III***

9:00 Paper 472c: Keynote Talk-Advanced Membrane Manufacturing for Water and Energy Applications — ***Oishi Sanyal***

9:30 Paper 472d: A Physics-Informed Machine Learning Model for Battery Capacity Fading Prediction with Early Cycling Data — ***Jiwei Yao***, *Qiang Gao, Benben Jiang, Kody Powell, Tao Gao*

9:45 Paper 472e: On Testing Methods for Image-Based Control Systems for Next-Generation Manufacturing — ***Henrique Oyama***, *Fnu Akkarakaran Francis Leonard, Katie Tyrrell, Helen Durand*

10:00 Paper 472f: Comparative Study for Evaluation of Thermal Integration Projects Based on Pinch Technology — ***Ícaro Almeida***, *Beatriz Dantas, Fernanda Andrade, Heloyse Reges, Wilton Lima, Fernando V. Lima,* ***Heleno Bispo***

10:15 Paper 472g: Dynamic Characteristics Investigation and Control of Tubular Reactor with Supercritical Water Gasification — ***Cui Wang***, *Hui Jin, Zhe Wu*

(473) Recycling and Upcycling of Plastic Waste

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, N-121A

Robert Peters, Chair
Raymond Smith, Co-Chair
Lucas Ellis, Co-Chair

Sponsored by: Waste Plastics

8:00 Paper 473a: A Techno-Economic and Life Cycle Analysis of Operating a Standalone Material Recover Facility in the United States. — ***Olumide Olafasakin***, *Sabrina Bradshaw, Horacio Aguirre-Villegas, Jiaze Ma, George Huber, Victor Zavala, Craig Benson, Mark Mba Wright*

8:12 Paper 473b: Techno-Economic Analysis and Life Cycle Assessment of Modular Microwave-Assisted PET Depolymerization — ***Yuqing Luo***, *Esun Selvam, Dionisios Vlachos, Marianthi Ierapetritou*

8:24 Paper 473c: Combining Chemical and Biocatalysis to Breakdown and Upcycle Polyethylene — ***Gwendolyn Gregory***, *Cong Wang, Sunitha Sadula, Raul Lobo, Dionisios Vlachos, Eleftherios Papoutsakis*

8:36 Paper 473d: Degradation of Polyethylene into Olefin Containing Products through Mechanochemistry — ***Laura Wilcox***, *Douglas P. Theberge, Yagnaseni Ghosh*

8:48: Break

9:00 Paper 473f: A Study of Metal Supported ZSM-5 and Y Zeolite for Microwave-Induced Degradation of Low-Density Polyethylene — ***Thang Luong***, *Yuxin Wang, Sean Brown, Jianli Hu*

9:12 Paper 473g: Impact of Acid Modified DBU-Based Ionic Liquids As Catalysts on Glycolysis of Poly (ethylene terephthalate) — ***Fahimeh Forouzeshfar***, *Maria Coleman, Joseph Lawrence*

9:24 Paper 473h: Microwave-Enhanced Catalytic Upcycling of Polymer — ***Yuxin Wang***, *Jianli Hu*

9:36 Paper 473i: Post-Consumer HDPE Waste Conversion to Lubricants: Techno-Economic Analysis and Life Cycle Assessment — ***Vincenzo Cappello***, *Pingping Sun, Guiyan Zang, Shishir V Kumar, Ryan Hackler, Hernán E. Delgado, Amgad Elgowainy, Massimiliano Delferro, Theodore Krause*

9:48 Paper 473j: Environmental Benefits of the Solvent-Targeted Recovery and Precipitation (STRAP) Process for Multilayer Plastic Films Recycling — ***Aurora Del Carmen Munguia Lopez***, *Dilara Goreke, George Huber, Victor Zavala*

10:00 Paper 473k: Production of Macronutrients from Hybrid Thermal and Biochemical Conversion of Waste Plastic — ***Jessica Brown***, *Efrain Rodriguez-Ocasio, Tannon Daugaard, Ryan Smith, Laura R. Jarboe, Robert Brown*

10:12 Paper 473m: Implement a Circular Ecomony for Plastic Waste in Developing Countries — ***Jeffrey Seay***, *Dimitrios Karadimas, Shelby Browning, Kaitlyn McGlennon*

(474) Thermal Energy Storage

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, N-227B

Gus Georgeton, Chair
Ravindra Aglave, Co-Chair

Sponsored by: Transport and Energy Processes

8:00 Paper 474a: Molecular-Level Understanding of Phase Stability in Model Phase-Change Nano-Emulsions for Thermal Energy Storage Investigated By NMR Spectroscopy — *Jungeun Park, Ulrich Scheler,* ***Robert Messinger***

8:25 Paper 474b: Development of Phase Change Material for Low Temperature Based Thermal Energy Storage Application — ***Kamal Nayan***

(475) John M. Prausnitz AIChE Institute Lecture

Wednesday, Nov 16, 11:15 AM
Phoenix Convention Center, North Ballroom 120D

Sindee Simon, Chair
De-Wei Yin, Co-Chair

Sponsored by: Awards Committee

11:15 Paper 475a: From Silicon to Plastic: It's All About Surfaces, Interfaces and Processing — ***Elsa Reichmanis***

(476) Biomass Conversion II: Carbon-Carbon Coupling & Redox Chemistry

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-128A

Ana Alba-Rubio, Chair
George Tsilomelekis, Co-Chair

Sponsored by: Catalysis

12:30 Paper 476a: Hydrogenation Kinetics of Biomass-Derived Monomers over Transition Metal Catalysts: Combined First-Principles and Experimental Study — ***Michael Rebarchik***, *Manos Mavrikakis, James A. Dumesic*

12:48 Paper 476b: Optimization of Aqueous Phase Furfural Hydrogenation Using Pd_1Ni Dilute Limit Alloy Catalysts — ***Md Fakhruddin Patwary***, *Leandro De Castro, Christopher Williams, John Regalbuto*

1:06 Paper 476c: Controlling Aldolization over Mg-Al Mixed Oxides Derived from Alkali-Free Layered Double Hydroxides — *Davi Petrolini, Ho-Yi Lam, Prashant Deshlahra,* ***Nathaniel Eagan***

1:24 Paper 476d: Ethanol Upgrading to Olefins over Metal-Containing Beta Zeolites: Characterization and Catalysis — *Nohor Samad,* ***Shivangi Borate****, Junyan Zhang, Michael Cordon, Evan C. Wegener, Stephen Purdy, Kinga A. Unocic, Dongxia Liu, Andrew D. Sutton, Zhenglong Li, James W. Harris*

1:42 Paper 476e: Cross-Ketonization of Biomass-Derived Furans and Fatty Acids for Renewable Surfactants — ***Tejas Goculdas****, Sunitha Sadula, Dionisios Vlachos*

2:00 Paper 476f: Catalytic Conversion of Lignocellulosic Carbohydrates into Drop-in Liquid Hydrocarbons — *Odiri Siakpebru, Prashant Niphadkar, Anoop Uchagawkar, Vijay Bokade, Bala Subramaniam,* ***Ana Colaco Morais***

2:18 Paper 476g: Probing the Performance and Mechanism of Nickel Iron Oxyhydroxides for Electrocatalytic Benzyl Alcohol Oxidation in Alkaline Media — ***Lingze Wei****, Michael Boyd, Md Delowar Hossain, Jaime Aviles Acosta, Melissa Kreider, Michaela Burke Stevens, Michal Bajdich, Thomas Jaramillo, Christopher Hahn*

2:36 Paper 476h: Competing Dehydration Reactions of Branched Alcohols on Solid Acid Catalysts — ***Mackenzie Todd****, Thomas Schwartz*

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(477) Data Science & Machine Learning Approaches to Catalysis II: AI-Accelerated Modeling of Catalysts and Materials

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-128B

Zachary Ulissi, Chair
Florian Goeltl, Co-Chair

Sponsored by: Catalysis

12:30 Paper 477a: AI-Accelerated Materials Modeling for Catalyst Discovery — ***Nongnuch Artrith***

1:06 Paper 477b: Finding Needles in a Haystack: Sifting through 16M Catalysts for Optimal Methane-to-Methanol Catalyst Design Under Weak Thermodynamic Scaling — ***Aditya Nandy****, Heather Kulik*

1:24 Paper 477c: Finetuna: Fine-Tuning Accelerated Molecular Simulations — ***Joseph Musielewicz****, Xiaoxiao Wang, Tian Tian, Zachary Ulissi*

1:42 Paper 477d: Investigations of Electric Field Effects on Catalysis: A Combination of Deep Learning Models and Multi-Scale Simulations — *Mingyu Wan, Han Yue, Hongfu Liu,* ***Fanglin Che***

2:00 Paper 477e: Machine Learning Predictions of Novel Ammonia Synthesis Catalysts Using Experimental and Literature Data — ***Withana A R Jayarathna****, Jochen Lauterbach*

2:18 Paper 477f: Integrating Experimental and Theoretical Data for High Quality Predictions of Electrocatalytic Performance — ***Shyam Deo****, Melissa Kreider, Michaela Burke Stevens, Kirsten Winther, Johannes Voss, Frank Abild-Pedersen, Thomas Jaramillo*

2:36 Paper 477g: First-Principles Analysis of the Ammonia Decomposition Reaction on High Entropy Alloycatalysts — ***Zuhal Cakir****, Liangbing Hu, Chao Wang, Jeffrey Greeley*

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(478) Electrocatalysis II: Catalyst and Characterization

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-127C

Marcel Schreier, Chair
Ezra Clark, Co-Chair
Jason Bates, Co-Chair

Sponsored by: Catalysis

12:30 Paper 478a: Understanding and Characterizing a Novel Cell Design for the Electrooxidation of Cyclohexene Towards Value Added Chemicals — ***Adrien Deberghes III****, Linsey Seitz*

12:48 Paper 478b: Is Electrification of the Manufacturing of Commodity Chemicals to Decarbonize Manufacturing Economically Feasible? — ***Nishithan Balaji Chidambara Kani****, Meenesh Singh*

1:06 Paper 478c: In-Situ Structure Dependent Water Oxidation Activity on Iridium Oxide Single Crystal Surfaces — ***Ankita Morankar****, Zhenhua Zeng, Jeffrey Greeley*

1:24 Paper 478d: Examination of a Hybrid Catalytic System for Electrochemical Reduction of CO_2 — ***Foroogh Khezeli****, Rezwanul Islam, Craig Plaisance*

1:42 Paper 478e: Effect of pH on the Electrocatalytic Oxidation of Glycolic Acid — ***Mohammad Hasan****, Ian McCrum*

2:00 Paper 478f: Tuning the Electronic Metal-Support Interaction to Design Stable and Active Oxygen Reduction Electrocatalysts — ***Kah Meng Yam****, Asmee Prabhu, Lavie Rekhi, Luan Q. Le, Tej Choksi*

2:18 Paper 478g: Hybrid Organic-Inorganic Interfaces Drive CO_2 Reduction to C_2 hydrocarbons — ***Mingyu Wan****, Zhiyong Gu, Fanglin Che*

2:36 Paper 478h: An Atomic-Scale View for Electrocatalysis — *Manos Mavrikakis,* ***Michael Rebarchik***

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(479) In Honor of Mark Barteau's Birthday (Invited Talks)

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-127B

James Medlin, Chair
Suljo Linic, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

12:30 Paper 479a: Data-Driven Acceleration of Catalyst Modeling — *Mingjie Liu, Yilin Yang,* ***John Kitchin***

12:52 Paper 479b: Controlling Selectivity in Reactions of Complex Oxygenates over Metal Catalysts — ***James Medlin***

1:14 Paper 479c: Surface Science of Metal Oxides – Insight into Structure-Activity Relationships through Studies of Single Crystals — ***John Vohs***

1:36 Paper 479d: Catalytic Performance Descriptors from First-Principles — ***Manos Mavrikakis***

1:58 Paper 479e: Kinetic and Spectroscopic Studies of Oxygen Reduction Reaction on Nonmodel Pt Electrocatalysts — ***Suljo Linic***

2:20 Paper 479f: Applications of Synchrotron Techniques for *in Situ* Catalytic Studies — ***Jingguang G. Chen***

2:42 Paper 479g: Forgotten Works — ***Mark Barteau***

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(481) Modeling and Analysis of Chemical Reactors II

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-223

Hanyu Gao, Chair
Behnam Partopour, Co-Chair

Sponsored by: Reaction Engineering

12:30 Paper 481a: Modeling of Fluid-Solid Heat and Mass Transfer in Particle Resolved CFD Simulations of Catalytic Fixed Bed Reactors — ***Martin Kutscherauer****, Sebastian Böcklein, Scott D. Anderson, Gerhard Mestl, Thomas Turek, Gregor D. Wehinger*

12:48 Paper 481b: Reactor Design and Optimization of α-Amino Ester Hydrolase for Synthesis of Cephalexin — ***Colton Lagerman****, Martha Grover, Ronald Rousseau, Andreas Bommarius*

1:06 Paper 481c: Verifying Properties of Chemical Reactors Using an Automated Theorem Prover — ***Parivash Feyzishendi****, Sophia Hamer, Jinyu Huang, Tyler R. Josephson*

1:24: Break

1:42 Paper 481e: Multi-Objective Catalyst Shape Optimization for Solid-Catalyzed Gas-Phase Reactions with q-Expected Hypervolume Improvement Via Particle-Resolved CFD Simulations — ***Woojin Kang****, Yesong Lee, Jonggeol Na, Wonbo Lee*

2:00 Paper 481f: A Spectro-Kinetic-Hydrodynamic Workflow to Assess Gas-Solid Operando Spectroscopic Cells As Intrinsic Kinetic Reactors — *Jose Valecillos, Héctor Vicente, Gorka Elordi, Mengmeng Cui, Ana Gayubo, Andres Aguayo,* ***Pedro Castano***

2:18 Paper 481g: Smart Reactor Design for Chemical Processes: Integrated CFD and Artificial Intelligence-Based Optimization Approach — ***Sungwon Hwang***

2:36 Paper 481h: Multiobjective Optimization of Resid Fluidized Catalytic Cracking Unit through Data-Driven Approach — ***Anubha Agrawal***, *Manoj Ramteke*

(482) Practical Applications of Computational Chemistry and Molecular Simulation for Solvents and Inorganic Materials

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-222B

Andrea R. Browning, Chair
Steven G. Arturo, Co-Chair
Sukrit Mukhopadhyay, Co-Chair
Christopher Muhich, Co-Chair
Jonathan Moore, Co-Chair
Martin Sanborn, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

12:30 Paper 482a: Mechanochemical Degradation Pathways of Protective Oxide Surfaces: Development of an Ab-Initio Informed Multiscale Corrosion Model — ***Jeremy Scher***, *Tae Wook Heo, Yue Hao, Matthew Kroonblawd*

1:00 Paper 482b: Molecular Insights into NMR Relaxation of Gd(III)-Based Contrast Agents for MRI Applications — ***Thiago Jose Pinheiro Dos Santos***, *Arjun Valiya Parambathu, Dilip Asthagiri, Philip Singer, Walter Chapman*

1:20 Paper 482c: Interface Force-Field (IFF) Parameterization of $Ti_3C_2T_X$ Mxenes — ***ISAAC Armstrong***, *Vikas Varshney, Hendrik Heinz*

1:40 Paper 482d: Molecular Characterization of High Ionic Conductivity in Fluoroether Lithium Metal Battery Electrolytes — ***Yuxi Chen***, *Elizabeth Lee, Juan J. de Pablo*

2:00 Paper 482e: Ab Initio Study on the Reaction Kinetics of Ethylene Glycol Decomposition on Pt (111) and Pt_3sc (111). — ***Shedrack G. Akpe***, ***Hyung Chul Ham***

2:20 Paper 482f: Oxidation Rate and Leaching of Flame-Made Nanosilver By Reactive Molecular Dynamics — ***Eirini Goudeli***, *Diego Chaparro*

2:40 Paper 482g: Molecular Dynamic Insights on the Distinct Solvation Structures of Aromatic and Aliphatic Compounds in Monoethanolamine Based Deep Eutectic Solvents — ***Nikhil Kumar***, *Tamal Banerjee*

(483) Design and Operations under Uncertainty - II

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, W-101C

Ana I. Torres, Chair
Can Li, Co-Chair

Sponsored by: Systems and Process Operations

12:30 Paper 483a: Dynamic Real-Time Scheduling and Control Under Uncertainty — ***Daniela Dering De Lima Silva***, *Christopher Swartz*

12:48 Paper 483b: Parallel Solution of Optimal Gas Network Control Under Uncertainty — ***Michael Bynum***, *Lorenz Biegler, Carl Laird, Sakshi Naik, Robert Parker, John Siirola*

1:06 Paper 483c: Constrained Robust Bayesian Optimization of Expensive Black-Box Functions Under Uncertainty — ***Akshay Kudva***, *Farshud Sorourifar, Joel Paulson*

1:24 Paper 483d: Deep Reinforcement Learning to Address Uncertainties in Computational Molecular Design — *Bryan Tantisujjatham*, ***Abdulelah Alshehri***, *Fengqi You*

1:42 Paper 483e: Technology Prioritization for Biofuel Supply Chain Design Via Stochastic Optimization — ***Yifu Chen***, *Eric O'Neill, Christos Maravelias*

2:00 Paper 483f: Multi-Objective Optimization of Flexible Integrated Biorefinery Design — ***Yuqing Luo***, *Marianthi Ierapetritou*

2:18 Paper 483g: An End-to-End Design and System Integration for Biomanufacturing on Mars Under Uncertainty — ***Georgios Makrygiorgos***, *Aaron J. Berliner, Anthony Abel, Stefano Cestellos-Blanco, Jeremy Adams, Nishi Thapliyal, Amor Menezes, Peidong Yang, Douglas S. Clark, Adam P. Arkin, Ali Mesbah*

2:36 Paper 483h: Development of a Health Monitoring Framework Under Uncertainty for Supercritical Coal Power Plants Considering Material and Operational Uncertainties — ***Katherine Hedrick***, *Elijah Hedrick, Benjamin P. Omell, Stephen Zitney, Debangsu Bhattacharyya*

(484) Modeling, Estimation and Control Applications

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, W-101B

David Gay, Chair
Xunyuan Yin, Co-Chair

Sponsored by: Systems and Process Control

12:30 Paper 484a: Simultaneous Estimation of Soil Moisture and Hydraulic Parameters for Precision Agriculture: A Real Case Study — ***Bernard Agyeman***, *Erfan Orouskhani, Jinfeng Liu*

12:49 Paper 484b: Optimal Feedback Morphology Control of Amphiphile Self-Assembly Using Markov State Models: Numerical Studies and Experimental Validation — ***Silabrata Pahari***, *Shuhao Liu, Mustafa Akbulut, Joseph Kwon*

1:08 Paper 484c: An Integrated System Identification and Hybrid Model Predictive Control Strategy for Optimized Interventions for Physical Activity — ***Mohamed El Mistiri***, *Owais Khan, Daniel Rivera, Cesar Martin, Eric Hekler*

1:27 Paper 484d: Optimization-Based Estimation and Control of Renewable Energy-Powered Greenhouse Systems — *Patrick Hinkel*, ***Davood Babaei Pourkargar***

1:46 Paper 484e: Multiple Model Predictive Control of the Cardiovascular System Using Vagal Nerve Stimulation — ***Yuyu Yao***, *Mayuresh Kothare*

2:05 Paper 484f: Operation and Control of Spatial Atomic Layer Etching Process — ***Matthew Tom***, *Sungil Yun, Henrik Wang, Feiyang Ou, Gerassimos Orkoulas, Panagiotis Christofides*

2:24 Paper 484g: State and Parameter Estimation of Complex Dynamic Systems Using Nonlinear Grey Box Modeling: Application to an Industrial Steam Superheater System — ***Vivek Saini***, *Debangsu Bhattacharyya*

2:43 Paper 484h: Dynamic Modeling of Recirculating Aquaculture Systems with an Integrated Application of Nonlinear Model Predictive Control and Moving Horizon Estimation — *Sara Kamali, Valerie Ward*, ***Luis Ricardez-Sandoval***

(485) Process Design in Energy and Sustainability: towards a net zero carbon economy

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, W-101A

Kirti Yenkie, Chair
Can Li, Co-Chair

Sponsored by: Systems and Process Design

12:30 Paper 485a: Multiscale Optimization of Integrated Energy Systems Using Machine Learning Models for Market Interactions — ***Jaffer Ghouse***, *Jordan Jalving, Bernard Knueven, Xian Gao, Xinhe Chen, Damian Agi, Nicole Cortes, John Siirola, David Miller, Alexander Dowling*

12:47 Paper 485b: An Operational Optimization Approach for Supply Network Decarbonization for Energy-Chemical Co-Production — ***Yuhe Tian***, *Benjamin Akoh*

1:04 Paper 485c: Modeling the Mobility Transition - a Multi-Scale Approach — ***Rahul Kakodkar***, *Swaminathan Sundar, Funda Iseri, Efstratios N. Pistikopoulos*

1:21 Paper 485d: Evaluating Impacts of Carbon Taxes on the Economic Viability and Carbon Footprint of Plastic Production Pathways — ***Bo-Xun WANG***, *Victor Zavala*

1:38 Paper 485e: Optimization of Biomass to Fuels with Carbon Capture: Economic and Environmental Analysis — ***Caleb Geissler***, *Christos Maravelias*

1:55 Paper 485f: Development of an Interactive Software Tool for Designing Industrial Solvent Recovery Processes — ***Jake Stengel***, *Austin Lehr, Emmanuel Aboagye, John Chea, Kirti Yenkie*

2:12 Paper 485g: A Practical Perspective on CO_2 Electrolysis in View of Future Net-Zero Energy Systems — ***Omar J. Guerra***, *Ana Somoza Tornos, Hussain Almajed, Wilson A. Smith, Bri-Mathias Hodge*

2:29 Paper 485h: Process Design and Operation for the Flexible Electrification of Methanol Synthesis — ***Jiaze Ma***, *Michael Rebarchik, Manos Mavrikakis, George Huber, Victor Zavala*

2:46 Paper 485i: Electrified Ethane Cracking Reactor Design and Modeling — ***Cornelius Masuku***

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(486) ABET Updates and Insights (Invited Talks)

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, W-105A

Douglas Ludlow, Chair
Randy S. Lewis, Co-Chair
Thomas Spicer III, Co-Chair
Tamara Floyd-Smith, Co-Chair
Donald Visco Jr., Co-Chair

Sponsored by: Undergraduate Education

12:30: Introductory Remarks

12:35: Presentation and discussion

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(487) ChE Summer School Highlights (Invited Talks)

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, W-105B

Daniel Burkey, Chair
Milo Koretsky, Co-Chair

Sponsored by: Education

12:30: Welcoming Remarks

12:45: Panel discussion: Planning committee

1:15: Panel discussion: Workshop presenters

1:45: Panel discussion: Summer school attendees

2:15: Concluding Remarks

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(489) Directed and Self Assembly of Colloids

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-232C

Bhuvnesh Bharti, Chair
Isaac Torres Diaz, Co-Chair
Po-Yen Chen, Co-Chair

Sponsored by: Interfacial Phenomena

12:30 Paper 489a: Nobel Metal Ion-Directed Assembly of 2D Materials for Synergistic Photocatalysts and Noble Metal Structuring — ***Joshua Little***, *Jiayue Sun, Leah K Borden, Umesha Dissanayake, Deborah Essumang, Benita Oseleononmen, Dongxia Liu, Taylor J. Woehl, Po-Yen Chen*

12:45 Paper 489b: Controlling the Nucleation and Growth of DNA-Programmed Colloidal Crystallization — ***W. Benjamin Rogers***

1:00 Paper 489c: Effects of Hydrodynamics on Self-Assembly of Nanoparticles — ***Jaehun Chun***, *Elias Nakouzi, Christopher J. Mundy, Gregory Schenter*

1:15 Paper 489d: Self-Assembly of Active Microcrystallites and Spinning Free Janus Particles — ***Amir Nourhani***, *Seyed Amin Nabavizadeh, John Castañeda, John Gibbs*

1:30 Paper 489e: Electric-Field Assembly of Two-Dimensional Colloidal Quasicrystals — ***Ning Wu***, ***Joseph Maestas***, *David Wu, David Wu*

1:45 Paper 489f: Long-Range Transport and Directed Assembly of Charged Colloids Under the Coupling of AC Electric Fields and Induced Concentration Gradients — ***Kun Wang***, *Samuel Leville, Behrouz Behdani, Carlos Silvera Batista*

2:00 Paper 489g: Assembly of Colloidal Clusters with Homochirality Under Combined Electric and Magnetic Fields — ***Xingrui Zhu***, *Joseph Maestas, David Wu, Ning Wu*

2:15 Paper 489h: Colloidal Isomerism Via Competing Interactions — *Hashir Gauri, Ahmed Al Harraq*, ***Bhuvnesh Bharti***

2:30 Paper 489i: Buckling of a Drying Drop of Colloidal Dispersion: Theory — ***Mahesh S. Tirumkudulu***

2:45 Paper 489j: Buckling of a Drying Drop of Colloidal Dispersion: Experiments — ***Om P. Bamboriya***, *Mahesh S. Tirumkudulu*

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(490) Dynamic Processes at Interfaces

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-232B

Samaneh Farokhirad, Chair
Esteban Urena-Benavides, Co-Chair

Sponsored by: Interfacial Phenomena

12:30 Paper 490a: Impact of Janus Particle Amphiphilicity on the Rheological Properties of the Air/Water Interface — ***Elton Lima Correia***, *Dimitrios Papavassiliou, Sepideh Razavi*

12:45 Paper 490b: Dynamics of Suspensions of Rotating Magnetically-Assembled Chains of Janus Particles — ***Jinghui Gao***, *Samuel Wilson-Whitford, James Gilchrist*

1:00 Paper 490c: Surface Viscoelasticity Hinders the Instabilities in Confined Multiphase Flows — ***Jiayu Li***, *Harishankar Manikantan*

1:15 Paper 490d: Mechanistic Insight into Decrease in Lung Surfactant Modulus As Acute Respiratory Distress Progresses — ***Clara Ciutara***, *Sourav Barman, Steven Iasella, Joseph Zasadzinski*

1:30: Break

1:45: Break

2:00 Paper 490g: Chaotic Dynamics of an Autophoretic Particle — *R Kailasham*, ***Aditya Khair***

2:15 Paper 490h: Dynamics of Chains and Disks Formation in Superparamagnetic Colloids Submitted to Magnetic Fields in Different Configurations — ***Geoffroy Lumay***, *Alexis Darras, Florence Mignolet*

2:30 Paper 490i: Pinning, De-Pinning and Stair-Case Hysteresis in Wetting of Porous Solids — ***Abhishek Kumar Barnwal***

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(491) Lithium & Beyond: Fundamental Advances in High Performance Batteries I

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-231A

Alexander Urban, Chair
Nian Liu, Co-Chair
Vilas G. Pol, Co-Chair
Theresa Schoetz, Co-Chair

Sponsored by: Electrochemical Fundamentals

12:30 Paper 491a: Diamond ATR-FTIR for in Situ Characterization of SEI Formation at the Lithium Metal Interface — ***Jeffrey Lopez***

12:50 Paper 491b: Understanding Electrochemical Discharge and Degradation Mechanisms in Li-CF_x Batteries from the Atomic to Macroscopic Scales — ***Loleth Robinson***, *Theresa Schoetz, Leo Gordon, MChem, MPhil, Robert Messinger*

1:10 Paper 491c: Lithium Superionic Conductivity and Interfacial Stability in Newly Predicted Li-Sulfide Battery from Reaxff — ***Tridip Das***, *Sergey I Morozov, Boris Merinov, Sergey Zybin, MoonYoung Yang, William Goddard III*

1:30 Paper 491d: Effects of Amino Thiophenol Additives on the Solid-Electrolyte Interphase in Lithium-Sulfur Battery — ***Zhao Wang***, *Wenduo Zeng, K.Y. Simon Ng*

1:45 Paper 491e: Interfacial Electrolyte Structure with Anti-Reductive Solvent at Electrode for Practical Lithium-Sulfur Batteries: A Molecular Dynamics Study — *Yiling Nan*, ***Zhehui Jin***

2:00 Paper 491f: Silicon/Carbon Nanofiber/Nanoparticle Composite Anodes for Li-Ion Batteries — *John Waugh, Abhishek Mondal, R. Wycisk*, ***Peter Pintauro***

2:15 Paper 491g: Optimization of Hydrogels for Non-Spillable Zn|MnO_2 Rechargeable Batteries Allowing for 2nd Electron MnO_2 Cycling — ***Jungsang Cho***, *Damon E. Turney, Gautam Yadav, Michael Nyce, Timothy Lambert, Sanjoy Banerjee*

2:30 Paper 491h: Atomistic Simulations of Ion Mobilities in Lithium-Ion Batteries — ***Pramudit Tripathi***, *Scott T. Milner*

2:45 Paper 491i: Thermodynamic Modeling of Non-Equilibrium Solidification of the Lithium Silicate System By Considering Mixed Kinetic Phenomena — *Sanchita Chakrabarty, Haojie Li,* ***Michael Fischlschweiger***

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(492) Microfluidic and Microscale Flows: Multiphase and Fields

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-231C

Alexandra Bayles, Co-Chair
Ankur Gupta, Co-Chair

Sponsored by: Fluid Mechanics

12:30 Paper 492a: Centrifugal Assembly of Helical Fibers for pH Responsive Composite Hydrogels — ***Shankar Kharal***, *Martin F. Haase*

12:45 Paper 492b: Architecting Soft Materials Using Fluidic Gates: A Practical Analogy to Boolean Logic — ***Alexandra Bayles***, *Tazio Pleij, Matthew Murdock, Jan Vermant*

1:00 Paper 492c: *Formation of Pixelated Elastic Films Via Capillary Suction of Curable Elastomers in Templated Hele-Shaw Cells* — ***Pierre-Thomas Brun***, *Christopher Ushay, Joel Marthelot, Grace Kresge, Mohamed Badaoui*

1:15 Paper 492d: Fabrication of Drug Loaded PLGA Microparticles Using a Microfluidic Flow-Focusing Device for Sustained Release Formulations — ***Nelia Viza***

1:30 Paper 492e: Diffusiophoresis in Zwitterionic Gradients — ***Parth Shah***, *Rodrigo Nery Azevedo, Todd Squires*

1:45 Paper 492f: Microfluidic Networks for Sorting of Drops: Design of Network Topology and Entry Times of Drops — ***Arun Sankar Eenhakkattu Mana***, *Raghunathan Rengaswamy*

2:00 Paper 492g: Electroviscous Effects in Electrolyte Liquid Flow through Asymmetrically Charged Contraction-Expansion Microfluidic Devices — ***Jitendra Dhakar***, *Ram Prakash Bharti*

2:15 Paper 492h: Coupling between Internal Dynamics and Transport of Polyelectrolytes in External Electric and Flow Fields — ***Dmitry I. Kopelevich***, *Jason E. Butler*

2:30 Paper 492i: Effect of Surfactants on Elongated Bubbles in Rectangular Capillary Channels: Liquid Encapsulation and Bursting — ***Paula Pico***, *Lyes Kahouadji, Assen Batchvarov, Seungwon Shin, Jalel Chergui, Damir Juric, Omar K. Matar*

2:45 Paper 492j: Two-Dimensional Diffusiophoretic Banding of Colloidal Particles — *Ritu Raj,* ***Ankur Gupta***

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(493) Nonlinear Flows and Combined Transport Processes

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-232A

Michael Howard, Co-Chair
Henry Chu, Co-Chair

Sponsored by: Fluid Mechanics

12:30 Paper 493a: Helicity and Dissipation Along the Trajectories of Passive Particles in Anisotropic Turbulent Fields — ***Oanh Pham***, *Dimitrios Papavassiliou*

12:45 Paper 493b: Enhancing Population Balance Models for Accurate Prediction of Bubble Size Distribution (BSD) in Column Reactors — ***Malik Hassanaly***, *John Parra-Alvarez, Hari Sitaraman*

1:00 Paper 493c: Prediction of Particle Dynamics Using Random Forcing Model in a Turbulent Particle-Laden Shear Flow — ***Partha Goswami***, *Swagnik Ghosh, V Kumaran*

1:15 Paper 493d: Turbulence Collapse in a Dilute Particle-Gas Suspension — ***V Kumaran***, *Partha Goswami, Pradeep Muramulla*

1:30 Paper 493e: Turbulence and Interpenetrating Continua, Part II — ***Charles Petty***, *Andre Benard*

1:45 Paper 493f: Discovery of Maximum Drag Enhancement Asymptote in Turbulent Flow of Dilutepolymeric Solutions — *Yabiao Zhu, Nansheng Liu,* ***Bamin Khomami***

2:00 Paper 493g: Peeling of Linearly Elastic Sheets Using Complex Fluids at Low Reynolds Numbers — ***Anirudh Venkatesh***, *Vishal Anand, Vivek Narsimhan*

2:15 Paper 493h: *Driving Force and Pathway in Polyelectrolyte Complex Coacervation* — ***Shensheng Chen***, *Zhen-Gang Wang*

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(494) Thermophysical Properties and Phase Behavior II

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-222C

Erik Santiso, Chair

Sponsored by: Thermodynamics and Transport Properties

12:30 Paper 494a: Efficient Implementation of Wertheim's Theory: II. Master Equations for Asymmetric Solvation — ***J. Richard Elliott***

12:48 Paper 494b: A Simple Method to Predict and Interpret the Formation of Azeotropes in Binary Systems Using Conventional Solvation Free Energy Calculations — ***Andrew Paluch***

1:06: Break

1:24 Paper 494d: Development of a Machine Learning Algorithm to Predict Diverse System Solubility — ***Rakshit Jain***, *Shubhajit Sen, Jacqueline Hughes-Oliver, Ronald Baynes, Erik Santiso*

1:42 Paper 494e: Investigation of Tuning Effect By Tetrahydrofuran (THF) in THF-H_2 Hydrates Via Molecular Dynamics Simulations — ***Dong Woo Kang***, *Wonhyeong Lee, Yun-Ho Ahn, Jae Lee*

2:00 Paper 494f: Formation Kinetics and Flow Behavior of Semi-Clathrate Hydrate Slurry in a Flow Loop: Application for Cold Energy Transport and Distribution — ***Junjie Zheng***, *Hyunho Kim, Ponnivalavan Babu, Praveen Linga*

2:18: Break

2:36 Paper 494h: Solubility Measurements of Coumarin Derivatives in Selected Organic Solvents — ***Hiroyuki Matsuda***, *Yuka Miyahara, Yuya Tashiro, Kiyofumi Kurihara, Katsumi Tochigi*

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(495) Fundamentals and Applications for Municipal Solid Waste Treatment and Valorization

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-225A

Matthew Alexander, Chair
Enoch Nagelli, Co-Chair
Mohamed Mostafa, Co-Chair
Robert Peters, Co-Chair

Sponsored by: Solid and Hazardous Waste

12:30 Paper 495a: Techno-Economic and Environmental Analysis of the Conversion of Food Waste to Renewable Energy — ***Yunzhi Chen***, *Elizabeth Grace Pinegar, Kody Powell*

12:55 Paper 495b: Resource Recovery from Solid Waste Anaerobic Digester - Performance, Energy Consumption and Cost — ***Yupo J. Lin***, *Deepak Dugar, Christopher W. Simmons*

1:20 Paper 495c: Predicting the Role of Reactive Nitrogen Intermediates during Hydrothermal Liquefaction of Food Waste — ***Heather LeClerc***, *Rasha Atwi, Amy M. McKenna, Michael T. Timko, Richard H. West, Andrew R Teixeira*

1:45 Paper 495d: Processes to Enable Full Material Recovery from Municipal Solid Waste — ***Tommy John***

2:10: Break

2:35 Paper 495f: Decentralized Anaerobic Digestion Waste-to-Energy System for Food Waste Treatment and Fertilizer Production at East Coast Lagoon Food Village (ECLFV) — ***Yong Wei Tiong***, *Pooja Sharma, Yen Wah Tong*

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(496) Sustainable Fuel from Renewable Resources

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-225B

Alvaro Orjuela, Chair
Juan-Gabriel Segovia-Hernandez, Co-Chair
Selen Cremaschi, Co-Chair
Shweta Singh, Co-Chair

Sponsored by: Sustainability

12:30 Paper 496a: Recent Advances in Intensification of Bio-Based Processes By Ultrasound and Hydrodynamic Cavitation — ***Yusuf Adewuyi***

12:55 Paper 496b: Glycerol As a Co-Solvent for Hydrothermal Liquefaction of Corn Stover — ***Khang Huynh***, *Bharathkiran Maddipudi, Anuradha Shende, Rajesh Shende*

1:20 Paper 496c: A Study of Trace Ammonia Impurities in Renewable Natural Gas and Their Impact on Its Potential Utilization — ***Linghao Zhao***, *Zhuofan Shi, Jingwen Gong, Jorge Gutierrez, Siari Sosa, Theodore Tsotsis*

1:45 Paper 496d: Multi-Scale Modelling of Low-Temperature Electrolysis of Steam in Molten Carbonate Cells — ***Maria Anna Murmura***, *Luca Turchetti, Maria Cristina Annesini*

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(497) Drug Delivery for Applications in the Brain, Nervous System, and Musculoskeletal System

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-126A

Handan Acar, Chair
Jessica Larsen, Co-Chair
Whitney Stoppel, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

12:30 Paper 497a: Branched-Tail Lipid Nanoparticles Potently Deliver mRNA across Multiple Murine Models — ***Mariah Arral***, *Pooja Pandya, Namit Chaudhary, Saigopalakrishna Yerneni, Kathryn Whitehead*

12:48 Paper 497b: Image-Guided, Bioactive Gas Delivery with Ultrasound-Activatable Microbubbles for Treatment of Ischemic and Traumatic Injuries — ***Rajarshi Chattaraj***, *Misun Hwang, Chandra Sehgal, Daniel A. Hammer, Daeyeon Lee*

1:06 Paper 497c: PLG Microparticles for Small Molecule Delivery to Muscle Cells — ***Candice Cheung***, *Kidochukwu Atube, Michael Gower*

1:24 Paper 497d: Highly Tunable Fluorescent Nanoparticle Library for Optimizing Neuronal Drug Delivery — ***Rachel Pollard***, *Parker Lewis, Dane Jensen, Rocco Latorre, Shlok Paul, Brian Schmidt, Nigel Bunnett, Nathalie M. Pinkerton*

1:42 Paper 497e: Brain-Derived Extracellular Vesicles: Molecular Probes and Therapeutic Vehicles in the Neonatal Ischemic Brain — ***Nam Phuong Nguyen***, *Hawley Helmbrecht, Elizabeth Nance*

2:00 Paper 497f: Nano-Hitchhikers for Effective Delivery of Alpha-Particle Radiotherapy to Glioblastomas — ***Rajiv Ranjit Nair***, *Tony Wu, Anjali Sharma, Rangaramanujam Kannan, Stavroula Sofou*

2:18 Paper 497g: Invited Talk: Placeholder for Invited Talk in the Drug Delivery for Applications in the Brain, Nervous System, and Musculoskeletal System Session — ***Whitney Stoppel***, *Handan Acar, Jessica Larsen*

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(498) Engineering bacteria for novel chemistry and interactions

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-125B

Jorge A. Marchand, Chair
John Blazeck, Co-Chair

Sponsored by: Bioengineering

12:30 Paper 498a: Engineering Embden-Meyerhof-Parnas (EMP) Glycolysis to Generate Noncanonical Reducing Power — *Edward King, Youtian Cui,* ***Derek Aspacio***, *Frances Nicklen, Linyue Zhang, Sarah Maxel, Ray Luo, Justin Siegel, Erick Aitchison, Han Li*

12:48 Paper 498b: *De Novo* Biosynthesis of the Non-Standard Amino Acid *Para*-Nitrophenylalanine — ***Neil Butler***, *Sabyasachi Sen, Minwei Lin, Aditya Kunjapur*

1:06 Paper 498c: Computational Design of CRISPR Guide RNAs to Enable Strain-Specific Control of Microbial Consortia — *Austin Rottinghaus,* ***Tae Seok Moon***

1:24 Paper 498d: A Workflow for the Systems-Level Analysis, Design, and Engineering of Genomically Recoded Organisms — ***Anush Chiappino-Pepe***, *Lisa Dratva, Courtney A. Shearer, Huseyin Tas, Jorge A. Marchand, Kamesh Narasimhan, Russel V. Miranda, Alexandra I. Rudolph, George M. Church*

1:42 Paper 498e: Circuit-Host Interactions: Mechanism and Control — ***Xiaojun Tian***

2:00 Paper 498f: Deregulating Native Bacterial Genetic Circuits As a Potential Anti-Microbial Therapeutic — ***William Bothfeld***, *Brian F. Pfleger*

2:18 Paper 498g: Engineered Microbes for Environmental Monitoring and Remediation — ***Ariel Furst***

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(499) Metabolic Engineering for Food, Feed, and Bioproducts

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-126B

Jie Dong, Chair
Blaise Kimmel, Co-Chair
Tae Seok Moon, Co-Chair

Sponsored by: Food

12:30 Paper 499a: Screening of a Combinatorial Pathway Library to Improve Isobutanol Production in *Saccharomyces Cerevisiae* — ***Joshua Dietrich***, *Francesca Gambacorta, Brian F. Pfleger*

12:48 Paper 499b: Metabolic Engineering of *Paraburkholderia Sacchari* for Improved Bioplastic Co-Polymer Production. — ***Dianna Morris***, *Cheryl Immethun, Mark Wilkins, Rajib Saha*

1:06 Paper 499c: Engineering a Mixotrophic Clostridium Consortium Directly Exchanging Cellular Materials Via Cell Fusion for Biochemical Production with CO_2 Fixation. — ***Hyeongmin Seo***, *Jonathan Otten, Noah Willis, John Hill, Eleftherios Papoutsakis*

1:24 Paper 499d: Metabolic Engineering of *Clostridium Tyrobutyricum* for Increased Intracellular NADH Pool and High-Yield *N*-Butanol Production — ***Jun Feng***, *Jialei Hu, Shang-Tian Yang*

1:42: Break

2:00 Paper 499f: Dynamic Regulation of 4-Hydroxycoumarin Synthesis in Engineered *Escherichia coli* — ***Yusong Zou***, *Jianli Zhang, Jian Wang, Yajun Yan*

2:18 Paper 499g: [Keynote] Systems and Synthetic Biology: Constructing Smart and Programmable Microbes to Address Global Problems — ***Tae Seok Moon***

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(500) Metabolic Platform Development- Non-Conventional Species and Systems

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-125A

Kevin Solomon, Chair
Eric Young, Co-Chair

Sponsored by: Bioengineering

12:30 Paper 500a: Cell-Free Biosynthesis to Inform Metabolic Engineering of Non-Model Bacteria — ***Blake J. Rasor***, *Ashty S. Karim, Michael Koepke, Michael C. Jewett*

12:48 Paper 500b: Engineering *Vibrio Natriegens* for Degrading and Assimilating Poly(ethylene terephthalate) — ***Tianyu Li***, *Nathan Crook*

1:06 Paper 500c: Engineering *Deinococcus Radiodurans* for Improved Nanoparticle Biosynthesis Using Small RNAs — ***Angela Chen***, *Julia Hernandez-Vargas, Runhua Han, Orlando Cortazar-Martinez, Natalia Gonzalez, Sonia Patel, Benjamin K. Keitz, Gabriel Luna-Barcenas, Lydia Contreras*

1:24: Break

1:42 Paper 500e: Integrative Omics Analysis of *Yarrowia Lipolytica* for the Bioconversion of Lipid-Based Substrates — ***Alyssa M. Worland***, *Zhenlin Han, Jeffrey Czajka, Yinjie Tang, Wei Wen Su*

2:00 Paper 500f: Investigating the Role of pBBR1's Mobilization Protein in Plasmid Maintenance in Non-Model Bacteria — ***Mark Kathol***, *Cheryl Immethun, Dianna Morris, Rajib Saha*

2:18 Paper 500g: Development of Non-Model Microbes As Chassis Organisms for Bioconversion — ***Adam Guss***

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(501) Sustainable Biodegradable Polymers from Renewable & Waste Resources

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-228A

Bandaru V. Ramarao, Chair
Deepak Kumar, Co-Chair

Sponsored by: Forest and Plant Bioproducts Division

12:30 Paper 501a: Microbial Upcycling of Post-Consumer Polyethylene Waste into Protein-Based Materials — ***Alexander Connor***, *Mattheos Koffas, Runye Zha*

12:43 Paper 501b: Development of Bioplastic: Need of the Hour — ***Rahul Taskar***, *Abhishek Yadav, Dr. Utkarsh Maheshwari*

12:56 Paper 501c: Renewable Barrier Polymers from Carbohydrate Nanomaterials: Processing and Properties — *Yue Ji, Yang Lu, Meisha L. Shofner, Tequila Harris,* ***J Carson Meredith***

1:09 Paper 501e: Evaluating Sustainable Alternatives for Membrane Separation Processes: The Case of Poly Hydroxy Alkanoates (PHA) — *Kseniya Papchenko, Eleonora Ricci,* ***Maria Grazia De Angelis***

1:22 Paper 501f: Synthesis of Thermoplastic Polyesters from Betulin, a Birch Bark-Derived Triterpenoid, Via Melt Polycondensations — ***Alexandra M. Lehman-Chong***, *Casey L. Cox, Joseph Stanzione III*

1:35 Paper 501g: Biodegradable Composite Films from Carbohydrate Rich Food Waste Streams: Physicochemical Properties, Scale up Production, and Biodegradability — *Shu Xu, Chaoyi Ba,* ***Meltem Urgun-Demirtas***

1:48 Paper 501h: Coproduction of Polyhydroxyalkanoates and Carotenoids By a Red Yeast Strain — *Krishanthi Mapa Mudiyanselage,* ***Caixia Wan***

2:01: Break

2:14 Paper 501j: The Integrated Production of Biopolymers, Monomers, and Electricity from Cheap Carbon Sources Using Microbial Fuel Cell Systems — ***Jianfei Wang***, *Shijie Liu*

2:27 Paper 501k: Feedstock Design for High-Quality Biomaterial Manufacturing — *Cheng Hu, Qiang Li, Arthur Ragauskas, Scott Sattler, William Rooney,* ***Joshua Yuan***

2:40 Paper 501i: Synthesis of Lignin-Based Polyesters — ***Hoyong Chung***, *Sundol Kim*

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(502) New processes for efficient CO2 capture and utilization under mild conditions

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-230

Andrew Tong, Chair
Kevin Whitty, Co-Chair

Sponsored by: Green Process and Product Engineering

12:30 Paper 502a: Developing Models to Understand Performance Trends of Electrochemically-Mediated Carbon Capture Systems — ***Lauren Clarke***, *Fikile R. Brushett*

1:00: Break

1:30 Paper 502c: Microwave Regeneration of CO_2 Solid Sorbent for Energy-Efficient Direct Air Capture — ***Gyoung Gug Jang***, *Diana Stamberga, Radu Custelcean, Costas Tsouris*

2:00 Paper 502d: Techno-Economic and Life-Cycle Assessment of Electrochemical Captured CO_2 Conversion Process in Monoethanolamine — ***Suhyun Lee***, *Woong Choi, Jae Hyung Kim, Yun Jeong Hwang, Jonggeol Na*

2:30 Paper 502e: Molecular Dynamics Studies on Separation of CO2/CH4 By the Ionic Liquids Encapsulated ZIF-8 — ***Lei Liu***

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(503) Process Intensification and Modular Manufacturing: Modeling and Simulation

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-221B

Fadhil Y. Al-Aboosi, Chair
Ignasi Palou Rivera, Co-Chair

Sponsored by: Process Intensification & Modular Chemical Processing

12:30 Paper 503a: Process Modeling and Simulation of Electrochemical Processes — ***Sadia Saberin***, *Chau-Chyun Chen*

12:50 Paper 503b: Production of Dimethyl Ether from Coal Using Chemical Looping: Process Simulation and Exergy Analysis — *Fanhe Kong, Qiaochu Zhang,* ***Pinak Mohapatra***, *Andrew Tong, Liang-Shih Fan*

1:10 Paper 503c: A Study on Capacity Expansion Scenarios of Intensified Ethylene Oxide Process — ***Chinmoy Basak Mukta***, *Selen Cremaschi, Mario Eden, Bruce J. Tatarchuk, Paul Dimick*

1:30 Paper 503d: Design of Intensified Reactor for Lean Methane Emissions Treatment — ***Adrian Irhamna***, *George M. Bollas*

1:50 Paper 503e: Dynamic Modeling and Explicit/Multi-Parametric Model Predictive Control Optimization of an Intensified Fluidized Bed Membrane Reactor for Oxidative Coupling of Methane — ***Moustafa Ali***, *Yuhe Tian, Shauvik De, Alexander P. van Bavel, C. Doga Demirhan, Efstratios N. Pistikopoulos*

2:10 Paper 503f: Modeling Water-Alcohol (C1-C3) Mixed-Solvent Electrolyte Solutions with Association Electrolyte Nonrandom Two-Liquid Activity Coefficient Model — ***Cheng-Ju Hsieh***, *Chau-Chyun Chen*

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(504) Emerging Junior Investigator Open Innovation Forum (Invited Talks)

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-228B

Jay Park, Chair
Younjin Min, Co-Chair
Jinhye Bae, Co-Chair
Won Tae Choi, Co-Chair

Sponsored by: International Committee

12:30 Paper 504a: Programmable Deformation and Instability of Responsive Hydrogels — ***Ji-Hwan Kang***

12:55 Paper 504b: Innovating Biomaterials Design for Precision Medicine in Biosensing — ***Jouha Min***

1:20 Paper 504c: Advancing the Fundamental Understanding of Redox-Driven Separations for Sustainable Water Desalination — ***Taeyoung Kim***, *Gowri Mohandass, Weikun Chen, Sitaraman Krishnan*

1:45 Paper 504d: Biosponge Polymer Membranes for Capturing Unwanted Toxins in the Body — ***Hee Jeung Oh***

2:10: Hanhwa Travel Award Flash Presentations

(505) Polymer Thermodynamics and Self-Assembly: Predicting Properties

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-121C

Reza Foudazi, Chair
Douglas Tree, Co-Chair
Zhe Qiang, Co-Chair
S. Eileen Seo, Co-Chair
Ian Hosein, Co-Chair
Melody Morris, Co-Chair

Sponsored by: Polymers

12:30 Paper 505a: Sustainable Thermoplastic Elastomers with Ionic Interactions — ***Megan Robertson**, Josiah Hanson, Wenyue Ding*

1:00 Paper 505b: Non-Trivial Phase Behavior of Ether-Based Block Polyzwitterions — ***Bradley Grim**, Frederick Beyer, Matthew D. Green*

1:15 Paper 505c: Phase Behavior and Mechanics of Triblock Copolymer Elastomers with Interaction-Tuned Additives — ***Karthika Madathil**, Bishal Upadhyay, S. Michael Kilbey II, Gila E. Stein*

1:30 Paper 505d: Polymer-Confined Nanoparticle Assembly with Interface Control — *Sayli Jambhulkar, **Kenan Song***

1:45 Paper 505e: Symmetry-Breaking in Patch Formation on Gold Nanoprism *Via* Supramolecular "Bandwagoning" — ***Thi Vo**, Ahyoung Kim, Hyosung An, Progna Banerjee, Lehan Yao, Shan Zhou, Chansong Kim, Delia Milliron, Sharon C. Glotzer, Qian Chen*

2:00 Paper 505f: Phase–Separation in Photopolymer Composite Media Under Non–Uniform Irradiation — ***Shreyas Pathreeker**, Ian Hosein*

2:15 Paper 505g: A Diblock Polymer Alloy Resulting in a C14 Phase Field — ***Ben Magruder**, Sojung Park, Ryan Collanton, Frank S. Bates, Kevin Dorfman*

2:30 Paper 505h: Using Sequence-Defined, Bioinspired Polymers to Understand Chain Conformation Effects in Block Copolymer Self-Assembly — ***Beihang Yu**, Scott Danielsen, PhD, Anastasia Patterson, Emily Davidson, Rachel Segalman*

2:45 Paper 505i: Chiral Conformations in Block Copolymers Affect the Thermodynamics of Self-Assembly — *Natalie Buchanan, **Poornima Padmanabhan***

(506) Polymers for Energy Storage and Conversion

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-122B

Santanu Kundu, Chair
Renxuan Xie, Co-Chair
Nese Orbey, Co-Chair
Rui Sun, Co-Chair

Sponsored by: Polymers

12:30 Paper 506a: Molecular Insights into Metal-Free Polymer Batteries — ***Jodie Lutkenhaus***

1:00 Paper 506b: Understanding Ion Transport in Single-Ion, Bottlebrush Copolymer Electrolytes through Experiments and Simulations — ***Zachary Brotherton**, Sanket Kadulkar, Venkat Ganesan, Thomas Truskett, Nathaniel Lynd*

1:15 Paper 506c: Design of a Boron-Containing Pthf-Based Solid Polymer Electrolyte for Sodium-Ion Conduction with High Na^+ Mobility and Salt Dissociation — *Francielli Genier, Shreyas Pathreeker, Paige Adebo, Paul Chando, **Ian Hosein***

1:30 Paper 506d: Thin Film Composite Separators for Energy Dense Lithium Batteries — ***Wyatt Tenhaeff***

1:45 Paper 506e: Ultra-Low Platinum Fuel Cells with Nanofiber/Nanoparticle Electrodes Produced *Via* simultaneous Needleless Electrospinning and Needle Electrospraying Technique — ***Dohyun Kim**, Yossef Elabd*

2:00 Paper 506f: Cyclic Carbonate-Based, Single-Ion Conducting Polymer Electrolytes for Li-Ion Batteries — ***Anthony Engler**, Habin PARK, Nian Liu, Paul Kohl*

2:15 Paper 506g: Side Chain Engineering of Conjugated Grafted Polymers for Electrochemical Transistors — ***Ashley Masucci**, Christian Pester, Enrique D. Gomez*

2:30 Paper 506h: Effect of Aging of P3HT Electrospinning Solution on the Processing Behavior and Fibers Properties — *Humayun Ahmad, **Santanu Kundu***

2:45 Paper 506i: Humidity-Dependent Mixed Ionic and Electronic Conduction of Conjugated Polyelectrolytes — *Garrett Grocke, **Shrayesh Patel***

(507) Sustainable and Bio-inspired composites

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-121B

Caroline Szczepanski, Chair
Colton Duprey, Co-Chair
Kailong Jin, Co-Chair

Sponsored by: Composites

12:30 Paper 507a: Multiscale Finite Element Simulation of Helically Symmetric Cellulose Nanocrystals in Alginate Fibers — ***Joshua Arp**, Christopher Kitchens*

12:50 Paper 507b: Recycling of Continuous Carbon Fibers from Thermoset Composites Using Joule Heating — ***Anubhav Sarmah**, Smita S. Dasari, Micah Green*

1:10 Paper 507c: Novel High-Performance Sustainable Biopolymer Films Hierarchically Reinforced with Dendricolloids — ***Yosra Kotb**, Orlin D. Velev*

1:30 Paper 507d: Bioinspired Nanocomposites for Next Generation Batteries — ***Ahmet Emre**, Emine Sumeyra Turali-Emre, Ji-Young Kim, Nicholas Kotov*

1:50 Paper 507e: Mesoporous, Moisture Absorbent, Temperature Controlled Hydrogelsfor Atmospheric Water Harvesting — ***Galen Mandes**, Jean-Francois Louf, Xiaohui Xu, Tapomoy Bhattacharjee, Rodney Priestley, Sankaran Sundaresan, Sujit Datta*

2:10 Paper 507f: All-in-One, Robust, Ready-to-Use, 3D Interconnected Hydrogels for Efficient Water Desalination — ***Shuaiming He**, Meng Ding, Wenhao Xu, Robin Park, Srinivasa R. Raghavan, Po-Yen Chen*

2:30 Paper 507g: Bioinspired Polydopamine Based Nanocomposite Coatings for Industrial Oily Water Treatment Membranes — ***Mohammad Hassan**, Moustafa Zagho, Shifa M. Shaikh, Mustafa Nasser, Xiaodan Gu, Sergei Nazarenko*

(508) Understanding Perovskite Semiconductors

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-122A

Letian Dou, Chair
Wiley Dunlap-Shohl, Co-Chair
Peijun Guo, Co-Chair

Sponsored by: Electronics and Photonics

12:30 Paper 508a: Thermomechanical Reliability of Halide Perovskite Semiconductors — ***Nick Rolston***

1:00 Paper 508b: Molecular Engineering Tailored Interface for Efficient and Stable Perovskite Solar Cells with Conducting Polymer — ***Ke Ma**, Jiaonan Sun, Letian Dou*

1:15 Paper 508c: 2D Halide Perovskites As Color-Changing Semiconductors — ***Jeffrey Christians**, Josephine Surel, Elizabeth Cutlip, James Mandeville*

1:30 Paper 508d: Elucidating the Relationship between Surface Chemistry of $CsPbX_3$ Perovskites and Their Transition Dipole Moment for Energy Transfer and Optoelectronics — ***Lindsey Parsons**, Carissa Eisler*

1:45 Paper 508e: Effects of 3D-Interfacial Strain on the Perovskite Phase Stability of $CsPbI_3$ in Silica Inverse Opal Scaffolds — ***Arkita Chakrabarti**, Aaron T. Fafarman*

2:00 Paper 508f: Perovskite to Non-Perovskite Phase Changes Using in Situ Measurements — *Jonathan Outen, Rory Campagna, Zachery R. Wylie, Riley Nelson, Samuel Smith, Bryce Grover, **Jeffrey Christians***

2:15 Paper 508g: Photoinduced, Reversible Phase Transition in Methylammonium Lead Iodide — ***Shunran Li**, Zhenghong Dai, Conrad Kocoj, Eric I. Altman, Nitin Padture, Peijun Guo*

2:30 Paper 508h: Unconventional Energy Transport Phenomena in Perovskite Nanomaterials — ***William Tisdale***

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(509) Bionanotechnology Graduate Student Award Session

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, W-105C

Lorraine Leon, Chair
Catherine Fromen, Co-Chair
Elizabeth Nance, Co-Chair

Sponsored by: Bionanotechnology

8:00 Paper 509a: Award Submission: Breast Cancer Specificity Assessment of Tumor Targeted Nano-, Encapsulated Manganese Oxide (NEMO) Particles — ***Celia Martinez de la Torre**, Dhruvi Panchal, Kasey Freshwater, Margaret Bennewitz*

8:20 Paper 509b: Award Submission: Single-Walled Carbon Nanotube Based NIR Sensors for Measuring Enzymatic Depolymerization of Polyurethanes — ***Mei-Tsan Kuo**, Jack Raffaelle, Nigel Reuel*

8:40 Paper 509c: Antibody-Free Rapid Detection of Sars-Cov-2 Proteins Using Corona Phase Molecular Recognition to Accelerate Development Time — ***Xiaojia Jin**, Sooyeon Cho, Xun Gong, Sungyun Yang, Jianqiao Leslie Cui, Michael Strano*

9:00 Paper 509d: Stable Anchorage of Inteleukin-12 Onto Layer-By-Layer Nanoparticles Enhances Immunotherapy of Metastatic Ovarian Cancer — ***Ivan S. Pires**, Darrell J. Irvine, Paula T. Hammond*

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(510) Nanoscale Science and Engineering Forum II (All Papers)

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, W-104B

Yoonjee Park, Chair
Yeongseon Jang, Co-Chair

Sponsored by: Nanoscale Science and Engineering Forum

12:30 Paper 510a: Detection and Classification of Chiral Inorganic Particles in Electron Microscopy Images Using Generalizable Deep Learning Algorithms — ***Anastasiia Visheratina**, Alexander Visheratin, Prashant Kumar, Michael Veksler, Nicholas Kotov*

12:49 Paper 510b: Association Rule Mining of the Relationships Among Biological Responses of Embryonic Zebrafish Exposed to Nanoparticles — ***Bilal Khan**, Yoram Cohen*

1:08: Break

1:27 Paper 510d: Evaluation of Nucleation and Growth Kinetics of Ionic Liquid-Based Pt Nanoparticles Synthesis in a Millifluidic Reactor By in Situ Small-Angle X-Ray Scattering — ***Majed Madani**, Noah Malmstadt*

1:46 Paper 510e: A First Step Towards the Development of a Nano-Production Line Using Multidisciplinary Quality By Design Approaches — ***Ramona Jeitler**, Carolin Tetyczka, Christina Glader, Bianca Brandl, Daniela Fiedler, Eva Roblegg*

2:05 Paper 510f: Surface Mineralization of Barley Stripe Mosaic Virus Biotemplates — ***Che-Yu Chou**, Yu-Hsuan Lee, Kok Zhi Lee, Chamath Vindula Basnayake Pussepitiyalage, Akash Vaidya, Shohreh Hemmati, Kevin Solomon, Sue Loesch-Fries, Michael T. Harris*

2:24 Paper 510g: *In-Vivo* Fluorescent Nanosensor Implants Based on Hydrogel-Encapsulation: Minimization of Inflammation and the Foreign-Body Response — *Michael A. Lee, **Xiaojia Jin**, Sureshkumar Muthupalani, Naveed Bakh, Michael Strano*

2:43 Paper 510h: 3D-Printed Graphene/Polymer Structures for Electron-Tunneling Based Devices — ***Deisy Cristina Carvalho Fernandes**, Vikas Berry, Philippe Poulin*

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(511) Novel, Unconventional, or Non-CSTR Mixing Systems

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-227C

Aaron Strand, Chair
Otute Akiti, Co-Chair

Sponsored by: North American Mixing Forum

12:30 Paper 511a: Residence Time Distributions, Turbulence, and Reactor Design — ***Christopher Tyler***

12:55: Break

1:20 Paper 511c: Solid-Liquid Flow and Mixing in Fluidic Oscillator — *Ketan Madane, **Vivek V. Ranade***

1:45 Paper 511d: Hydrodynamics Characterisation in a Three-Phase Flotation System Using Positron Emission Particle Tracking (PEPT) — ***Pablo Brito-Parada**, Diego Mesa, Katie Cole, Michael R. van Heerden*

2:10 Paper 511e: Utilization of Readily Available Computer Programs for Design of Fluid Mixing Equipment — ***W. Roy Penney***

2:35 Paper 511f: Detecting Lagrangian Coherent Structures in Twin-Screw Extruder Elements Via Smoothed Particle Hydrodynamics — ***Hannes Bauer**, Johannes G. Khinast*

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(512) Particle Technology Forum Award Presentations and Baron Award Lecture (Invited Talks)

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-229AB

Ben Freireich, Chair

Sponsored by: Particle Technology Forum

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(513) Advances in New Modalities: Predictive Modeling Technologies

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-123

Xiaoxiang Zhu, Chair
Moiz Diwan, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

12:30 Paper 513a: Integrated Model-Based Design and Scale-up for Peptide Chromatographic Purification — ***Bhoja Kandela**, Bent Colin, Shekhar Viswanath*

12:51 Paper 513b: Model-Aided Reaction Kinetics and Rheology Study of Solid Phase Peptide Cleavage Process — ***Jingyao Wang**, **Lexie Niemoeller**, Shekhar Viswanath, Yu Lu, Michael Kobierski, Bradley M. Campbell*

1:12: Break

1:33 Paper 513d: Coarse-Grained Molecular Dynamics Simulation of Aggregation and Surface Adsorption of ssDNA Loaded Adeno-Associated Viral Capsids — ***Tibo Duran**, Arani Chanda, Willow DiLuzio, Ryan Bellucci, Shivangi Naik, Bodhisattwa Chaudhuri*

1:54 Paper 513e: Leveraging Molecular Modeling in the Selection of Protein-Drug Candidates for Late-Stage Developability — ***Marco Blanco**, Francis Insaidoo, Jainik Panchal, Veronica Juan, Marc Bailly*

2:15 Paper 513f: Design of Experiments Compared to Artificial Neural Network Approach – How Can We Use Them to Understand Spray Drying of Biologics? — ***Daniela Fiedler**, Elisabeth Fink, Isabella Aigner, Eva Roblegg, Johannes G. Khinast*

2:36 Paper 513g: Investigating Fundamental Motions to Rapidly Predict Lyophilized Protein Stability — ***Kelly Badilla***, *Andreas Bommarius, Marcus T Cicerone*

(514) Panel Session: Pre-competitive Collaborations Through The Enabling Technologies Consortium (ETC)

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-124AB

Nandkishor Nere, Co-Chair
Daniel Patience, Co-Chair
Jean Tom, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

12:30: Opening Remarks by Nandkishor Nere/ Daniel Patience

12:35 Paper : Introduction to ETC — ***James M. Vergis***

12:45 Paper : Emerging Microfluidic Platforms for Crystallization Process Design: From Academic Research to Commercialization through ETC — ***Meenesh Singh***

12:57 Paper : The Compact HPLC Project: A Collaboration between Axcend and the Enabling Technologies Consortium — ***Ray West***

1:09 Paper : Next Generation Models for Crystal Morphology Prediction – a Collaboration between ETC & Ucsb — ***Michael F. Doherty***

1:21 Paper : Development of the online HPLC with the ETC — ***Vaso Vlachos***

1:33 Paper : User-Friendly Population Balance Model with Data Integration for the Digital Design of Crystallization Systems — ***Zoltan Nagy***

1:45: Break

1:55: Panel Discussion

1:57: Leadership Panel Discussion with Shailendra Bordawekar (AbbVie), Jean Tom (BMS), Aaron Cote (Merck), Vaso Vlachos (Autochem), Jason Tedrow (Sanofi) and Deepak Jain (Zoetis)

2:57: Concluding Remarks

(515) Pharma 4.0 (Advanced Controls, Process Automation, Data Analytics, etc.) in Drug Substance and Drug Product I

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-122C

Dominique Hebrault, Chair
Dana Barrasso, Co-Chair
Hossein Salami, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

12:30 Paper 515a: Development of a Flow Platform for Autonomous Model-Based Experimental Design — ***Christopher Hone***, *Sebastian Knoll, Clemens E. Jusner, Peter Sagmeister, Jason Williams, Martin Horn, C. Oliver Kappe*

12:51 Paper 515b: Machine Learning-Assisted Autonomous Reactor Characterization: Mass Transfer Coefficients for Oxidative Biocatalytic Reactions — ***Ajit Vikram***, *Keith A. Mattern, Shane T. Grosser*

1:12 Paper 515c: Optimization-Based Approaches for Explainable, Automated Chemometric Models — ***Chrysoula Kappatou***, *James Odgers, Salvador Garcia Munoz, Ruth Misener*

1:33 Paper 515d: Automated Process in Continuous Pharmaceutical Manufacturing through Real-Time Process Monitoring and Disturbance Detection Using PAT and Online First-Principle Models — ***Yuma Miyai***, *Nathan Puryear, Roudabeh Sadat Moazeni Pourasil, Cameron Armstrong, Taylor Raine, Rachel Vallejo, Sherif Abdelwahed, Thomas Roper*

1:54 Paper 515e: ML-Ops Platforms and Cloud Computing in Pharmaceutical Development — ***Jose Tabora***

2:15: Break

2:36 Paper 515g: Digital Assets, Digital Threads, and Digital Twins for Rapid Commercialization of Medicines: A Reference Architecture and Implementation to Enable Pharma 4.0 — ***Pablo A. Rolandi***, ***Matt Potter-Racine***

(516) Experiences in Teaching Process Safety

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-221C

Kenneth Cox, Chair

Sponsored by: Product Design

12:30 Paper 516a: Process Safety Education: Moving Beyond the Obvious — ***Thomas Spicer III***

12:51 Paper 516b: Student Incident Reporting As a Tool for Hazard Reductions in Unit Operations (UO) Laboratories — *Samira Azarin,* ***Christopher Barr***, *Joanne Beckwith, Janie Brennan, Tracy Carter, Amy Karlsson, Sarah Wilson*

1:12 Paper 516c: Process Safety Instruction in Chemical Engineering at Purdue University — ***Ray Mentzer***

1:33 Paper 516d: Incorporation of Che Safety into the Core Curriculum — ***Taryn Bayles***, ***Robert Enick***

1:54 Paper 516e: Incorporation of Safety Instruction into the Chemical Engineering Undergraduate Curriculum at UMass Lowell — ***Eric L. Maase***, ***Glenn R. Dissinger***

2:15 Paper 516f: Learnings from Five Years of Collaboration between Academia and Industry on Delivering Process Safety Competency Development Programs for Process Safety Engineers. — ***Luc Vechot***, *Tomasz Olewski*

2:36 Paper 516g: Teaching Process Safety from Different Perspectives: Bringing Together Academics and Practicing Engineers to Improve Process Safety Instruction in Chemical Engineering. — ***Stephanie Loveland***, *Christopher Schemel*

(517) Materials and Processes for Water Purification and Desalination II

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-222A

Sitaraman Krishnan, Chair

Sponsored by: Product Design

12:30 Paper 517a: Adsorptive Membranes Incorporating Ionic Liquids (ILs), Deep Eutectic Salts (DESs) or Graphene Oxide (GO) for Metal Salts Extraction from Aqueous Feed — *Liyan Qalyoubi,* ***Ioannis Zuburtikudis***, *Hadil Abu Khalifeh, Enas Al Nashef*

12:55 Paper 517b: Modifying Surface Properties of Cation Exchange Membranes Utilizing Chitosan for Electrodialysis — ***Matthew Sheorn***, *Humayun Ahmad, Santanu Kundu*

1:20 Paper 517c: Exploring the Roles of Different Components of Biomass in the Biosorption of Heavy Metals in Wastewater — ***Junli Liu***, *Chunhua Zhang, Bernard Tao, Janna Beckerman*

1:45 Paper 517d: Scale Inhibition Performance of Newly Synthesized Biodegradable Polymers Vs Commercially Available Phosphonate Inhibitors — ***Nadhem Ismail***, *Ali Alshami*

2:10 Paper 517e: Factorial Design Evaluation of Acesulfame K, Irgasan and Caffeine Removal from Water Using Lignocellulosic Food Residues As Bioadsorptive Materials in Packed Bed Filtration — ***Andrés Lagos***, ***Andrea Landázuri***, *Lourdes Orejuela Escobar, Juan Proaño-Avilés*

2:35 Paper 517f: Comparative Study on Catanionic and Anionic Dyes Removal Using Carpentry Waste Derive Biosorbent — ***Payal Maiti***, *Bhim Charan Meikap*

(518) Advanced Inorganic Materials for Membrane Gas Separation

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-132A

Haiqing Lin, Chair
Seokjhin Kim, Co-Chair

Sponsored by: Membrane-Based Separations

12:30 Paper 518a: Carbon Molecular Sieve Hollow Fiber Membranes Derived from Dip-Coated Precursor Hollow Fibers Comprising Nanoparticles — ***Yuhe Cao***, *Kuang Zhang, Chen Zhang, William J. Koros*

12:51 Paper 518b: Tailoring Molecular Structures of Hybrid Carbon Molecular Sieve Membranes for Natural Gas Processing — ***Hyun Jung Yu***, *Jong Suk Lee*

1:12 Paper 518c: Ceramic-Carbonate Hollow Fiber Membranes with Improved Mechanical Strength for High Temperature CO_2 Separation — *Tianjia Chen,* ***Jerry Lin***

1:33 Paper 518d: Moisture-Resistant Graphene-Based Nanolaminate Membranes for Hydrogen Purification Enabled By Charge Neutralizing Nanofillers — ***Behnam Ghalei***

1:54 Paper 518e: Novel Graphene Oxide-Based Membrane Structure for a Highly Effective Breathable Barrier for Toxic Vapors and Chemical Warfare Agents — *Yufeng Song, Cheng Peng, Zafar Iqbal,* ***Kamalesh Sirkar****, Gregory W. Peterson*

2:15 Paper 518f: Unexpected Gas Separation Selectivity in SSZ-13 Zeolite Membranes — *Ninad D. Anjikar, Orhan Talu, Qiang Fu, Sankar Nair,* ***Shaowei Yang***

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(519) Advanced Polymer Membranes for Gas and Vapor Separations

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-131B

Chen Zhang, Chair
Lingxiang Zhu, Co-Chair

Sponsored by: Membrane-Based Separations

12:30 Paper 519a: Effect of Co Ions in Cross-Linked Poly(ethylene oxide) on O_2 Transport Characteristics — ***Taliehsadat Alebrahim****, Narjes Esmaeili, Thien Tran, Haiqing Lin*

12:51 Paper 519b: Polyformamidine As Fixed-Site Carrier for CO_2/N_2 Separation Membranes — ***Jingying Hu****, Yang Han, Winston Ho*

1:12 Paper 519c: Transforming Barrier Polymers to High-Performance Gas Separation Membranes — ***Gaurav Iyer****, Chen Zhang*

1:33 Paper 519d: A Versatile Microporous Poly(Arylene Ether) Platform for Membrane-Based Gas Separation — ***Jing Ying Yeo****, Sheng Guo, Francesco Maria Benedetti, Duha Syar, Timothy Swager, Zachary Smith*

1:54 Paper 519e: Novel Iptycene-Based Polybenzimidazole Membranes for H_2/CO_2 Separation — ***Mengdi Liu****, Ruilan Guo*

2:15 Paper 519f: Thermal Cross-Linking of Ultra-Robust Membranes for Plasticization Resistance and Enhanced Permeability — ***Hyun Jung Yu****, Jong Suk Lee*

2:36 Paper 519g: Elucidating the Effect of Chlorination Versus Fluorination on the Transport Properties of Polymer Membranes for Gas, Vapor and Organic Solvent Separation — *Jing Deng, William Box, Lucas Condes, Yoshiyuki Okamoto,* ***Michele Galizia***

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(520) Characterization of Adsorbent Materials

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-131C

Li-Chiang Lin, Chair
Roger D. Whitley, Co-Chair

Sponsored by: Adsorption and Ion Exchange

12:30 Paper 520a: Advances in Surface Chemistry Assessment of Adsorbents By Combining Adsorption, Liquid Intrusion and NMR Spectroscopy — *Carlos Cuadrado Collados, Dorothea Wisser, Jakob Söllner, Markus Terlinden, Martin Hartmann,* ***Matthias Thommes***

12:48 Paper 520b: Brunauer-Emmett-Teller (BET) Surface Areas from Nitrogen and Argon Isotherms Are Similar — ***Yongchul G. Chung****, Archit Datar, Sunghyun Yoon, Li-Chiang Lin*

1:06 Paper 520c: Molecular Simulation of Adsorption and Diffusion in Rigid Nanoporous Amorphous Materials — ***Raghuram Thyagarajan****, David Sholl*

1:24 Paper 520d: Philippine Natural Zeolites and Its Potential for Air Quality Management — ***Bryan Alamani****, Jose Aldrin Vea, Eleanor Olegario, Ramuel John Tamargo*

1:42 Paper 520e: Advanced Characterization of Disordered Mesoporous Solids — ***Henry R. N. B. Enninful***

2:00 Paper 520f: Characterization of LTA Zeolites Based on Pore Typification — ***Sebastiao M. P. Lucena****, Jose Carlos A. Oliveira, Daniel V. Gonçalves, Diana C. S. Azevedo, Moisés Bastos-Neto*

2:18 Paper 520g: Post Spinning Modification of Porous Organic Cage Fiber Sorbents for CO_2 Capture — ***Isaiah Borne****, Jennel McGriff, Christopher W. Jones, Ryan P. Lively*

2:36 Paper 520h: The Use of Zeolites and Carbons for the Separation of Refrigerant R-410A: Thermodynamic Modeling of Pure Gas and Binary Sorption — ***Andrew Yancey****, David R. Corbin, Mark Shiflett*

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(521) Continuous Crystallization Processes

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-131A

Zoltan Nagy, Chair
Gerard Capellades, Co-Chair

Sponsored by: Crystallization and Evaporation

12:30: Introductory Remarks

12:33 Paper 521a: Development of Slug Flow Crystallization for Reactive Crystallization — *Mingyao Mou, Anna Berberoglu,* ***Consuelo Del Pilar Vega-Zambrano****, Huayu Li, Bing-Shiou Yang, Mo Jiang*

1:02 Paper 521b: Limitations and Optimization Potential of Continuous Chiral Resolution By Simultaneous Preferential Crystallization in Fluidized Bed Crystallizers — ***Jonathan Gänsch****, Nadiia Huskova, Heike Lorenz, Andreas Seidel-Morgenstern*

1:31 Paper 521c: Continuous API Salt Formation *Via* Sono-Msmpr Crystallization — ***Patrick Corona****, Benjamin M. Cohen*

2:00 Paper 521d: Slug Flow Reactor Simulation for Controllable Residence Time Distribution Using Computational Fluid Dynamics. — ***Chaeeun Lee****, Mingyao Mou, Mo Jiang, Jonggeol Na*

2:29 Paper 521e: Continuous Crystallization Process Development of Modafinil: A Step Towards Achieving Integrated Continuous Manufacturing — *Shailesh Agrawal, Jean-Christophe Monbaliu, Cornelis Vlaar, Jorge Duconge, Vilmalí López-Mejías,* ***Torsten Stelzer***

2:58: Concluding Remarks

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(522) Honorary Session for Prof. Ranil Wickramasinghe I

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-130

Cristiana Boi, Chair
Raja Ghosh, Co-Chair

Sponsored by: Bio Separations

12:30 Paper 522a: Opening Remarks — ***Cristiana Boi***

12:51 Paper 522b: Evaluation of Preferred Binding Orientations of Protein Therapeutics in Multimodal Chromatographic Systems Using Protein Fingerprinting and Dewetting Simulations — ***Steven Cramer***

1:12 Paper 522c: Electrochemical Separations for Bioprocessing Applications. — ***Sandra Kentish****, Qiuyue Wang, Sahar Talebi, George Chen*

1:33 Paper 522d: Developing an Electrospun Zwitterionic Membrane to Treat Produced Water Via Membrane Distillation — ***Jorge Almodovar***

1:54 Paper 522e: Virus Clearance during Downstream Purification of Protein Therapeutics — ***Xianghong Qian****, Solomon Isu, Ranil Wickramasinghe*

2:15 Paper 522f: High Performance Countercurrent Membrane Systems for Bioprocessing — ***Andrew Zydney***

2:36 Paper 522g: Multifunctional to Bioinspired Nanostructured Membranes — ***Dibakar Bhattacharyya****, Rollie Mills, Francisco Leniz, Lindell Ormsbee*

(523) Advances in Algae Cultivation, Conversion and Products

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-226B

Lynn Wendt, Chair
Sridhar Viamajala, Co-Chair

Sponsored by: Sustainable Biorefineries

12:30 Paper 523a: Algal-Based Bioremediation of Landfill Leachate — ***Thinesh Selvaratnam**, Hari Kharel, Melissa Tan*

12:48 Paper 523b: Applying Novel Mineral-Hydrogel Composites to Mitigate Harmful Algal Bloom and Supply Photo-Biorefineries — ***Zhengyang Xiao**, Albern Tan, Vincent Xu, Young-Shin Jun, Yinjie Tang*

1:06 Paper 523c: Investigation of Surfactant Aided Liquid Foam Photobioreactor for the Cultivation of Microalgae — ***Anuradha Krishnan**, Amarjeet Bassi*

1:24 Paper 523d: Photobiological Production of High-Value Compounds Via Compartmentalized Co-Cultures Using Ca-Alginate Hydrogels — ***Runyu Zhao**, Annesha Sengupta, Albern Tan, Taylor Pinkerton, Ryan Whelan, Young-Shin Jun, Himadri B Pakrasi, Yinjie Tang*

1:42 Paper 523e: Artificial Intelligence-Guided Bioprocess Design to Achieve Record Algal Productivity — *Bin Long, **Joshua Yuan***

2:00 Paper 523f: Critical Material Attributes of Algae Biomass for Successful Preservation in Storage Identified through Machine Learning Models — ***Bradley Wahlen**, Lynn Wendt, Chelsea St. Germain, Oluwatosin Oginni*

2:18 Paper 523h: Overcoming Engineering Challenges for the Hydrothermal Liquefaction of Cost-Advantaged Algal Feedstocks — ***Peter Valdez**, Scott Edmundson, Andrew J. Schmidt, Todd R. Hart, Dylan Cronin, Samuel P. Fox, Uriah Kilgore, Teresa Lemmon, Marie Swita*

(524) Advances in Clean Energy R&D (Invited Talks)

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-226C

Shweta Singh, Chair
Ashley Pennington, Co-Chair
Dharik Mallapragada, Co-Chair

Sponsored by: Sustainable Energy

12:30 Paper 524a: *Sustainable Process Systems Engineering As an Energy Transition Driver* — ***Antonis Kokossis***

1:00 Paper 524b: Closed Loop Systems for Critical Materials and Energy Transition — ***Maria Curry-Nkansah***

1:30 Paper 524c: Understanding How Hydrogen Fits into the Energy Future — ***Brittany Westlake***

2:00 Paper 524d: Outlook for Flexible CO_2 Capture Technologies for Meeting Grid Needs and Climate Goals — ***Stuart Cohen***

(525) Process Design: Innovation for Sustainability

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-226A

Vassilis Charitopoulos, Chair
Vikas Khanna, Co-Chair
Rui Shi, Co-Chair

Sponsored by: Sustainability Science and Engineering

12:30 Paper 525a: Experimental Study and Aspen Plus Simulation of Chemical Looping Gasification of Woody Chips Using Biochar-Based Oxygen Carrier — ***Shima Masoumi**, Lijun Wang*

12:45 Paper 525b: Process Simulation with Trees As Unit Operations for Improving Air Quality, Sequestering Carbon, and Reducing Cost — ***Yazeed Aleissa**, Bhavik Bakshi*

1:00 Paper 525c: Design and Environmental Assessment of an Ionic-Liquid-Based R407F Refrigerant Separation Process — *Daniel Jovell, Josep Oriol Pou Ibar, Rafael González-Olmos, **Felix Llovell***

1:15 Paper 525d: Decision Matrix Tool for Selection of Novel Solvents and Absorption Process Modifications to Improve the Performance of Post-Combustion CO_2 Capture — ***Daniel Bahamon**, Omar Khalifa, Ismail Alkhatib, **Lourdes Vega***

1:30 Paper 525e: Multi-Criteria Decision Support Tools for the Optimization of Input-Output Models for Industrial Symbiosis at the Point Lisas Industrial Estate, Trinidad — ***Thérèse G. Lee Chan**, Kyle Joshua, David A. Janes*

1:45 Paper 525f: Sustainability Assessments for Three High-Volume Chemical Processes — ***Matthew Alexander**, Christian Ogundipe, Nobby Acquah, Prince Tsegah*

(526) Engineering Cancer I: Mechanistic Studies

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-126C

Thomas Zangle, Chair
Blanca Quinones Diaz, Co-Chair

Sponsored by: Chemical Engineers in Medicine

12:30 Paper 526a: The Effects of Intratumoral Heterogeneity on Metastasis of Triple-Negative Breast Cancer Cells — ***Molly Brennan**, Susan E. Leggett, Sophia Martinez, Celeste M. Nelson*

12:48 Paper 526b: The Effects of Palmitate-Induced IRE1α Activation in DNA Double Strand Break Repair and the Development of Chemotolerant Breast Cancer Cells — ***Kevin Chen**, S. Patrick Walton, Christina Chan*

1:06 Paper 526c: Macrophages Aggregate and Cooperate to Phagocytose Cohesive Tumor Cell Targets in Engineered Immuno-Tumoroids and Solid Tumors — ***Lawrence J. Dooling**, Jason C. Andrechak, Brandon H. Hayes, Siddhant Kadu, Dennis E. Discher*

1:24 Paper 526d: Mechanistic Characterization of Homologous Recombination in BRCA2 Mutant Cancers — ***Shayne Sensenbach**, Prashant Karki, Mehmet Orman*

1:42 Paper 526e: Modeling Cancer Dormancy and Recurrence with the Theory of Birth-Death Processes — ***Adeyinka Lesi**, David Rumschitzki*

2:00 Paper 526g: Machine-Learning Based Prediction of Membranolytic Peptides with Anticancer Activities — ***Atefe Alimirzaei**, Christopher Kieslich, Hyeju Song*

2:18 Paper 526h: Caspase-Dependent HDAC4 Translocation Due to Microsecond Pulsed Electric Field (μsPEF) Exposure of Glioblastoma Cells — ***Zahra Safaei**, Gary Thompson*

(527) Interfacial Chemical Conversion

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-227A

David Flaherty, Chair
Peijun Guo, Co-Chair

Sponsored by: Material Interfaces as Energy Solutions

12:30 Paper 527a: Advancing Nondestructive *in Situ* Infrared Nanospectroscopy of Buried Electrochemical Interfaces in Li-Ion and Li-Metal Solid State Batteries — ***Robert Kostecki**, Hans Bechtel, Jonathan Larson, Xin He*

1:10 Paper 527b: Plasma-Liquid Interface for Promoting Organic Electrosynthesis without Solid Electrodes — *Xiaoshuang Chen, Aditya Ponukumati, Marcus Foston, **Elijah Thimsen***

1:25 Paper 527c: Harnessing Spontaneous Electric Fields to Direct Thermochemical Catalysis — *Thejas Wesley, **Yuriy Roman**, Yogesh Surendranath*

1:40 Paper 527d: Saponin-Based Surfactant: Chemistry, Properties, and Applications on Enhanced OIL Recovery – Towards Sustainability — ***Lourdes Orejuela Escobar**, Inés Hernández-Guerra, Juan Carlos Pereira, Yanet Villasana, Andrea Landázuri, Arleth Gualle Brito*

1:55 Paper 527e: Determining Solvation Energies for Aqueous-Phase Reaction Adsorbates Using Ab-Initio Molecular Dynamic Simulations — ***Ankita Morankar***, *Hee-Joon Chun, Zhenhua Zeng, Jeffrey Greeley*

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(528) Next-Gen Manufacturing in Pharma, Food, and Bioprocessing I

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-221A

Manjiri Moharir, Chair
Ravendra Singh, Co-Chair

Sponsored by: Next-Gen Manufacturing

12:30 Paper 528a: Process Design of a Fully Integrated Continuous Biopharmaceutical Process Using Economic and Ecological Impact Assessment — ***Chaoying Ding***, *Hiren D. Ardeshna, Christopher Gillespie, Marianthi Ierapetritou*

12:51 Paper 528b: An Integrated State Estimation, Covariance Estimation, and Optimal Control Framework of a Semi-Batch Reactor for Bioprocess Applications — ***Ronald Alexander***, *Marcelo P. A. Ribeiro, Fernando V. Lima*

1:12 Paper 528c: Hybrid Kinetic-Stoichiometric Model of CHO Cell Fed-Batch Process — ***Mariana Monteiro***, *Cleo Kontoravdi*

1:33 Paper 528d: Efficient Modeling of Critical Process Parameters in Bioreactors – a Case-Study across Scales — ***Johannes G. Khinast***, *Philipp Eibl, Christian Witz*

1:54 Paper 528e: Tablet Manufacturing Using Dried Whole Puerto Rican Sweet Potato and Breadfruit Particles — ***Luis Torrens-Sotomayor***, *Carlos Velazquez*

2:15 Paper 528f: Explainable One-Class Classification Neural Network Model for Tablet Quality Control — *Alex Taylor, Rob Holt,* ***Aycan Hacioglu***

2:36 Paper 528g: Closed-Loop Optimal Control Operation of an Industry-Scale Bioreactor and Experimental Validation — ***Parth Shah***, *M.Ziyan Sheriff, Mohammed Saad Faizan Bangi, Joseph Kwon, Costas Kravaris, Chiranjivi Botre, Junichi Hirota*

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(529) Sustainable Pathways to Clean Hydrogen and Synthetic Fuels IV

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, W-103B

William Gibbons, Chair
Eric Miller, Co-Chair

Sponsored by: Sustainable Pathways Toward Hydrogen and Synthetic Fuels

12:30 Paper 529a: Techno-Economic Evaluation of Carbon-Negative Hydrogen Production from Biomass — ***Mohammad Ostadi***, *Leslie Bromberg, Daniel R. Cohn, Emre Gençer*

12:55 Paper 529b: Hydrogen Production By Methane-Biomass Co-Pyrolysis — ***Haiyan Guo***

1:20 Paper 529c: Insights into Gas-Phase Methane Pyrolysis for Hydrogen Production and Carbon Capture — ***Patrick Lott***, *Manas B. Mokashi, Akash B. Shirsath, Heinz Müller, Corina Janzer, Steffen Tischer, Lubow Maier, Olaf Deutschmann*

1:45 Paper 529d: Methane Decarbonization for Hydrogen and Sequestered Carbon Nanofiber Co-Product — ***Jessica Hauck***, *Kent J. Warren, Linfei Li, Mija H. Hubler, Boning Wang, Andrew Broerman, Samantha Harshberger, Theodore Champ, Alan Weimer*

2:10 Paper 529e: Microwave-Assisted Dry Reforming of Methane — ***Sagar Sourav***, *Cong Wang, Weiqing Zheng, Dionisios Vlachos*

2:35: Break

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(530) Conversion of Waste Plastic into Liquid Fuels

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-121A

Shelby Browning, Chair
Lucas Ellis, Co-Chair
Robert Peters, Co-Chair

Sponsored by: Waste Plastics

12:30 Paper 530a: Effect of Acidic Pyrolyzed Hydrochar on Hydrothermal Liquefaction of Waste PVC — ***Vahab Ghalandari***, *Toufiq Reza*

12:51 Paper 530b: Catalytic Microwave-Assisted Pyrolysis of Plastic Waste for Fuels and Carbon Material — ***Leilei Dai Sr.***, *Roger Ruan Sr., Paul Chen, Yanling Cheng*

1:12 Paper 530c: Hydrothermal Liquefaction of Waste Plastics and Lignin — ***Sampath Gunukula***, *Sampath Karunarathne, Clayton Wheeler*

1:33 Paper 530d: Steam Catalytic Conversion of Waste Plastics into Fuels and Chemicals. — ***Foster Agblevor***, *Corey Skenandore, Hamza Abdellaoui, Ezra Johnson, Corbin Romney*

1:54 Paper 530e: The Chemistry and Kinetics of Polyvinyl Chloride (PVC) Pyrolysis — ***Jiayang Wu***, *Konstantinos Papanikolaou, Feng Cheng, Bennett Addison, Amy Cuthbertson, Gregg T. Beckham, Manos Mavrikakis, George Huber*

2:15 Paper 530f: Optimization of Waste Plastic to Fuel Oil Plants' Deployment Using Mixed Integer Programming(MIP) — ***David Muyise***

2:36 Paper 530g: Liquid-Fed Plastic Pyrolysis Pilot Plant: Effect of Reactor Volume on Product Yields — ***Daniel Kulas***, *Ali Zolghadr, David Shonnard*

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(531) Advanced Electrochemical Energy Storage Technologies I

Wednesday, Nov 16, 12:30 PM
Phoenix Convention Center, N-227B

Gang Wu, Chair
Ling Fei, Co-Chair
Shuya Wei, Co-Chair

Sponsored by: Transport and Energy Processes

12:30 Paper 531a: Structure and Dynamics of Water-in-Salt Litfsi Electrolytes from First-Principles Molecular Dynamics Simulations — ***Ramanish Singh***, *Xiaobo Lin, Yong Zhang, Edward Maginn, Peter Cummings, Joern Siepmann*

12:50 Paper 531b: Tuning Molecular Rigidity to Modulate Lithium Coordination and Enhance Mobility in Ionic Liquids — ***Matthew Gebbie***, *John McAlpine*

1:10 Paper 531c: High Energy Density Picoliter Batteries for Colloidal Robots and State Machines — ***Ge Zhang***, *Jing Fan Yang, Volodymyr Koman, Sungyun Yang, Allan Brooks, Matthias Kuehne, Michael Strano*

1:30: Intermission

1:50: Break

2:00 Paper 531e: Optimization and Surface Characterization of Porous Zinc Anodes for Zinc Metal Batteries — ***Matthew Powell***, *Shuya Wei*

2:20 Paper 531f: Hierarchical Multiphase Porous Electrode Theory -- a Case Study of Porous Graphite Electrode — ***Huada Lian***, *Martin Z. Bazant*

2:40 Paper 531g: Advanced Halogenated Electrolytes for Improved Performance, Safety, and Cycle Life of High Energy Lithium-Ion Batteries — ***Robert Emmett***

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(532) Poster Session: Catalysis and Reaction Engineering (CRE) Division

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, North Hall E

Thomas Schwartz, Co-Chair
Alyssa Hensley, Co-Chair
Shaama Mallikarjun Sharada, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

Poster 683d: Overcoming Propane Dehydrogenation Equilibrium Limitations Using a Catalyst/Membrane Hollow Fiber System — ***Rawan Almallahi***, *James Wortman, Suljo Linic*

Poster 532a: Continuous Carbon Recovery from HTL Aqueous Phase — ***Heather LeClerc***, *Geoffrey Tompsett, Daniele Castello, Michael T. Timko, Thomas H. Pedersen, Andrew R Teixeira*

Poster 532b: Applying Energy Conversion and Catalyst Rationale Towards Sustainability, Hydrogen Production and Nuclear Waste Management — ***Dylan Rodene***, *Edward Chandler, Ebtesam Eladgham, Katelyn Shell, Indika Arachchige, Ram Gupta, Frank Gupton*

Poster 532c: Morphology-Dependent Catalytic Activity of Wrinkled Silica Sphere Supported Palladium for One-Pot Furfural Hydrogenation — ***Yeeun Kim***, *Jae Ho Baek, Kwan-Young Lee, Man Sig Lee*

Poster 532d: Modification of Surface Acidity of Pd/TiO_2 Catalysts for Hydrogenation of Furfural — ***Hye Jin Song***, *Yeeun Kim, Jungho Jae, Man Sig Lee*

Poster 532e: Ketonization and Etherification Reactions for Sustainable Biomass Conversion — ***Chenyang Li***, *Rajeev Assary*

Poster 532f: Thermochemical Modulation on Boron-, Phosphorus-, and Sulfur-Containing Siliceous Zeolites for Renewable Tetrahydrofuran Dehydra-Decyclization to Butadiene — ***Raisa Carmen Andeme Ela***, *Gaurav Kumar, Manish Shetty, Xinyu Li, Wei Fan, Paul Dauenhauer*

Poster 532g: Synthetic Natural Gas Production Based on Steam Hydrogasification of Agriculture-Derived Waste Streams — ***Zhongzhe Liu***, *Chan Seung Park, Partho Roy, Xin Fan, Hugo Cortes Lopez, Danny Valtierra, Chloe Hansen, Marco Ceja, Rosely Ayala, Robert Lozano, Serina Ishida*

Poster 532h: Hydrotreatment of Soybean Oil for Green Fuels with Ni-Mo/Zeolite Y Catalysts — ***You-Lin Lin***, ***Bing-Hung Chen***

Poster 532i: Oxidation Kinetics of Fe Doped Magnesium Manganate Systems — ***Jayni Hashimoto***, *Alicia Bayon, Olivia Tamburro, Vivienne Pelletier, Christopher L. Muhich*

Poster 532j: Design of Bi-Functional Zeolite-Based Catalysts for Bio-Oil Upgrading into Fuels — *Abdulla Alhendi, Aasif Dabbawala, Kyriaki Polychronopoulou, Maryam Khaleel,* ***Seba AlAreeqi***

Poster 532k: Electrocatalytic Upgrading of Model Compounds Derived from Pyrolysis Oil — ***Jeffrey Page***, *Lei Yu, Stoyan Bliznakov, Julia A. Valla*

Poster 532l: Enhancing Activity of Ligand-Modified Supported Metal Catalysts for Hydrodeoxygenation — ***Zachary Blanchette***, *Daniel K. Schwartz, J. Will Medlin*

Poster 532m: *Valorization of Glycerol from the Biodiesel Industry to Obtain Oxygenated Additives* — *Silvia S. O. Silva, Matheus R. Nascimento,* ***Francisco Murilo Tavares de Luna***, *Celio Cavalcante Jr.*

Poster 532n: Investigating the Effect of Solvents over Brønsted Acid Sites of Zeolite Using Alkylamine Hofmann Elimination — ***Han Chen***, *Omar Abdelrahman*

Poster 532o: Elucidation of Reaction Kinetics between Supercritical Methanol and Cellulose-Derived 1,2-Propanediol for Biofuel Production — ***Raka G. Dastidar***, *George Huber, Michael Lanci, Chengrong Wang, Peter Galebach*

Poster 532p: Effect of Temperature and Pressure on CO_2 and Steam Gasification of Nigerian Biomass Char — *Funmilayo Osuolale,* ***Jieun Kim***, *Kevin Whitty*

Poster 532q: Production and Evaluation of Esterification Catalysts Based on Starch-Derived Mesoporous Carbons (Starbons®) Using Colombian Starches As Feedstock — ***Milena Zabala***, *Laura Panqueba, Alvaro Orjuela, Suranjana Bose, James Clark*

Poster 532r: In-Situ Operando and Ex-Situ Study on Light Hydrocarbon-like-Diesel and Catalyst Deactivation Kinetic and Mechanism Study during Deoxygenation of Sludge Oil — ***Alsultan Abdulkareem***, *Nurul Asikin Mijan, Robiah Yunus, Taufiq-Yap Yun Hin*

Poster 532s: Biomass Produces Glycolic Acid — ***Ziqi Zhou***, *Dongpei Zhang, Quanxing Zhang, Shengyan Ma, Xin Jin*

Poster 532t: Electromagnetic Catalysis for Fusion Pump Oil Detritiation — ***Alaba Ojo***, *John Regalbuto, Kori Mcdonald, George Larsen, Jay Gaillard, Tyler Guin, Mark Elvington, Prabhu Ganesan, Joseph Meany*

Poster 532u: Textile Wastewater Treatment Using Coiled Flow Inverter (CFI) As a Photo-Reactor — ***Kamal Nayan***, *Gunjan Kumar Agrahari*

Poster 532v: Hydrothermal Production of Microalgal Bio-Oil Intensified with Supercritical CO_2 and Carbon-Based Catalysts — ***Armando Quitain***, *Shunsuke Kimura, Jonas Karl N. Agutaya, Tetsuya Kida*

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Poster 532ab: Understanding the Mechanism of C-N Coupling in Electrochemical CO_2 Reduction on Metal Surfaces — ***Tianyou Mou***, *Xue Han, Huiyuan Zhu, Hongliang Xin*

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Poster 532af: Beyond Tafel Fitting for Kinetic Analysis of Electrochemical CO_2 Reduction — ***Kaitlin Corpus***, *Justin Bui, Aditya Limaye, Karthish Manthiram, Adam Weber, Alexis T. Bell*

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Poster 532ai: Impact of Pressure on Fuel Production Via Redox — ***Justin Tran***, *Kent J. Warren, Alan Weimer*

Poster 532aj: Surface Compositional and Chemistry Tuning of Ni-Zn Catalyst for Low-Temperature Dry Reforming of Methane. — ***Olusola Johnson***, *Yang He, Changyi Jiang, Babu Joseph, John Kuhn*

Poster 532ak: Ni-Doped $Ca_xTi_yO_3$ Perovskite As a Catalytic Sorbent for an Integrated CO_2 Capture and Subsequent Dry Methane Reforming — ***Seongbin Jo***, *Kandis Leslie Abdul-Aziz*

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Poster 532ar: Aqueous-Phase Heats of Adsorption of Phenolics in Mixed Electrolytes — ***Ankit Mathanker***, *Wendy Yu, Isaiah Barth, James Akinola, Nirala Singh, Bryan Goldsmith*

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Poster 532aw: Unraveling the Mechanisms of Electrocatalytical Reduction of Furfural Via Tailoring Interfacial Environments — *Hengzhou Liu, Deep M. Patel, Yifu Chen, Jungkuk Lee, Luke Roling,* ***Wenzhen Li***

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Poster 532ba: A General Route Towards Low-Methane Hydrogenolysis of Polyethylene over Ruthenium on Doped Zirconias at Mild Conditions — ***Cong Wang***, *Kewei Yu, Boris Sheludko, Tianjun Xie, Pavel Kots, Brandon Vance, Pawan Kumar, Eric A. Stach, Weiqing Zheng, Dionisios Vlachos*

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Poster 532bf: Bifurcation Analysis of the Oxidative Dehydrogenation of Ethane over M1 Phase Catalysts in Shallow Autothermal Reactor — ***Jiakang Chen***, *Praveen Bollini, Vemuri Balakotaiah*

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Poster 532bm: Regeneration Strategies to Maximize Catalyst Stability and Productivity for Methane Dehydroaromatization Via Periodic-Switch, Pulse Feeding, and Catalysts Integration — ***Mamoun Al-Rawashdeh***, *Anchu Ashok*

Poster 532bn: Tuning the Reactivity for Propane Dehydrogenation By Using Well-Defined, Single-Phase Pt-Sn Nano-Catalysts — ***Baraa Werghi***, *Amani Ebrahim, Miaofang Chi, Matteo Cargnello, Simon Bare*

Poster 532bp: The Role of Coo-Co Nanoparticles Supported on Silica in Fischer Tropsch Synthesis: Evidence of Enhanced CO Dissociation and Olefin Hydrogenation. — ***Nothando Shiba***, *Yali Yao, Xinying Liu*

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Poster 532br: Effect of Surface Oxidation of Cr2O3(0001) on Propane Dehydrogenation: A Multiscale Study — ***Matej Huš***, *Drejc Kopač, Damjan Lašič Jurković, Blaž Likozar*

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Poster 532bw: Optimization and Screening of Iron Supported on Clinoptilolite As a Low-Temperature Fischer- Tropsch Synthesis Catalyst — ***Roick Chikati***, *Joshua Gorimbo, Diakanua Nkazi*

Poster 532bx: Understanding the Formation of Possible Intermediate in MDA on Molycarbide Anchored over ZSM-5 and Effect of Light Hydrocarbons on Carburization of Mo in Mo/ZSM-5 Catalyst. — ***Iqra Ahangar***, *Sonit Balyan, M. Ali Haider, K.K. Pant*

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Poster 173ad: Hydrogen-Based Processing of Mineral Iron Carbonate; Iron Production Combined with Catalytic CO/CO_2 Hydrogenation — *Sascha Kleiber, Astrid Loder,* ***Matthäus Siebenhofer***, *Susanne Lux*

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Poster 532cc: Mechanistic Investigation of Electrochemical $C(sp^3)$–H Oxidation for the Late-Stage Methylation of Complex Amines — ***Kaida Liu***, *Matthew Neurock, Mayank Tanwar, Luiz F.T. Novaes, Song Lin, Justin S. K. Ho, Kaining Mao, Elisia Villemure, Jack A. Terrett*

Poster 532cd: Application of Hydrophobic Alkyl Ligand on Palladium Catalyst for Direct Synthesis of Hydrogen Peroxide — ***Seok-Ho Lee***, *Geun-Ho Han, Kwan-Young Lee*

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Poster 532cf: Understanding Electrocatalytic Phenomena Using Grand Canonical DFT — ***Abdulaziz Alherz***, *Nick Singstock, Charles B. Musgrave*

Poster 532cg: Investigation of Active Sites for Electrochemical Bromine Evolution Using Nitrogen-Doped Carbon Nanostructures — ***Dishari Basu***, *Jonathan Hightower, Deeksha Jain, Anne Co, Aravind Asthagiri, Umit Ozkan*

Poster 532ch: Highly Active Multifunctional Lanthanum Perovskite Electrocatalysts ($LaMn_xCo_{1-x}O_3$ ($0 \le x \le 1$)) By Tuning the Mn to Co Ratio in Alkaline Medium — ***Sadiyah Shafath***, *Khulood Logade, Anchu Ashok, Anand Kumar, Ibrahim Abu-Reesh*

Poster 532ck: Effects of Particle Addition on Sonochemical Degradation of Phenol — ***Daisuke Kobayashi***, *Miyu Moriyama, Mari Shiina*

Poster 532cl: Enhancing Epoxidation Activity with Hydrogen Peroxide over Highly Dispersed Tantalum Incorporated Mesoporous Silicates — ***Anoop Uchagawkar***, *Gustavo Barraza, Anand Ramanathan, Bala Subramaniam*

Poster 532cm: Facile Activation of Mixed Light Alkanes with Ozone in Pressure-Tunable Condensed Phases — ***Hongda Zhu***, *Timothy Jackson, Bala Subramaniam*

Poster 532cn: Catalytic Conversion of Methane to Methanol over Copper Ion-Exchanged MFI Type Zeolites — ***Venugopal Balashanmugam***, *Niket Kaisare, Parasuraman Selvam*

Poster 532co: Catalytic Surface Chemistry of Non-Noble Transition Metal Borides in the Selective Hydrogenation of Unsaturated Aldehydes and Nitro Compounds — ***Sijie Guo***, *Siris Laursen*

Poster 532cp: The Optimization in Catalysis Due to Better Adsorption to the Gold Surface within the SBA-15 Pores — ***Zengran Sun***, *Ellis Hammond-Pereira, Steven Saunders*

Poster 532cq: Impact of Pretreatment on the CeO_2 Structure and Catalytic Activity for CO Oxidation — ***Kyung-Min Lee***, *Taejin Kim, Gihan Kwon, Melanie Brito, Jamie DeCoster, Kelvin Linskens, Kareem Mehdi, Emily Kim, Hajoon Kim*

Poster 532cr: Density Functional Theory (DFT) for Selective Carboxylic Acid Hydrogenation on Ag, Cu-TiO_2 Catalysts — ***Jeremy Hu***, *Mikyung Hwang, Eun Mi Kim, Michael J. Janik, Hilal Ezgi Toraman, Konstantinos Alexopoulos*

Poster 532cs: Novel Kinetic Model for the Ethyl Acetate Synthesis By Direct Addition on a Silicotungstic Acid Catalyst. — *Bram Van Wettere,* ***Joris Thybaut***, *Erhin de Werd, Saleh Aghakhani, Jeroen Lauwaert*

Poster 173v: Role of Surface-Solvent Interactions on Alkene Epoxidation Catalysis within Ti-MFI — ***Chris Torres***, *David Potts, David Flaherty*

Poster 173ac: Condensed Phase Catalytic Conversion of Benzyl Alcohol to Phenol Using High-Frequency Ultrasound: A Combined Experimental and DFT Investigation — ***Shang Jiang***, *Teseer Bahry, Francois Jerome, Prince N. Amaniampong,* ***Samir H. Mushrif***

Poster 532ct: Enhancing Thermal Resistance and Performance of Three-Way Catalyst By Physical Mixing of Bimetallic Catalysts — ***Hyoseong Woo***, *Eun Jun Lee, Junki Yoo, Seorin Ji, Kwan-Young Lee*

Poster 532cu: Aqueous Phase Heats of Adsorption of Phenolics in Aqueous Environments: Role of Chaotropic and Kosmotropic Species — ***Wendy Yu***, *Ankit Mathanker, James Akinola, Isaiah Barth, Bryan Goldsmith, Nirala Singh*

Poster 532cv: Black Carbon across Decadal Length Scales: Biofuel Content Dependence — *Akshay Gharpure,* ***Randall Vander Wal***

Poster 532cw: Trends in Catalytic Activity of Single-Atom M/TiO_2 Catalysts Towards CO Oxidation — ***Liping Liu***, *Ayman M. Karim, Hongliang Xin*

Poster 532cx: Theoretical Methods for Assessing the Feasibility of PFOA Oxidation on Photo-Catalyst Surfaces — ***Yu Chen***, *Manav Bhati, Thomas Senftle*

Poster 532cy: Cu Loaded Hierarchical MFI Zeolite Synthesis and the Effect of Its Physicochemical Properties As Hydrocarbon Trap during Cold Start Test — ***Jinseong Kim***, *Jungkyu Choi*

Poster 532da: Catalytic Remediation of Chlorophenolic Compounds in Drinking Water: Understanding the Reaction Mechanism Using DFT Simulations — ***Chaitra Shenoy***, *Shelaka Gupta, Tuhin Suvra Khan, Mayank Agrawal, M. Ali Haider*

Poster 173w: Role of Co and Mn on Low-Temperature NO_x Adsorption Behaviors of Layered-Double-Hydroxide-Based Passive NO_x Adsorber — ***Yeji Choi***, *Ki Bong Lee*

Poster 532db: Classifying Zeolite Material Selection for O_2 Sorption Pump Materials Using Machine Learning and a Density Functional Theory — ***Steven Wilson***, *Zoe Liberman-Martin, Ellen B. Stechel, Christopher L. Muhich*

Poster 532dc: Sulfur-Trioxide Decomposition over β–SiC Foam Supported $CuFe_2O_4$ in the Sulfur-Iodine Cycle — ***Sachin Tomar***, *Sreedevi Upadhyayula*

Poster 532dd: The Critical Role of Hidden Basic Sites of Na-ZSM-5 in the Dehydration of Lactic Acid — *Jichan Kim*, ***Jungho Jae***

Poster 532de: Stabilizing Atomically Dispersed Cu for Low-Temperature Water-Gas Shift Reaction — ***Yiwei Yu***, *Jingyue Liu*

Poster 532df: Metal Incorporation into Zeolites *Via* Acid-Base Mediated Ion Exchange for Methane Dehydroaromatization — ***Jacek Pecyna***, *Md Sifat Hossain, Rob Hart, Sheima J. Khatib*

Poster 532dg: Manipulation of Amorphous Precursors to Enhance Zeolite Nucleation — ***Zhiyin Niu***, *Deependra Parmar, Yu Liang, Heng Dai, Jeffrey Rimer*

Poster 532dh: Programmable Catalysts Inspired By Semiconductor Devices — ***Sallye Gathmann***, *C. Daniel Frisbie, Paul Dauenhauer*

Poster 532di: Shape-Selective Silver Catalysts for Ethylene Epoxidation — ***Kaveh Shariati***, *Jochen Lauterbach*

Poster 532dj: Ionic Liquids Regulated La-Mn Composite Metal Oxides for Selective Oxidation of Cyclohexane — ***Hao Li***, *Ruixia Liu, Ruirui Zhang*

Poster 532dk: Gold Nanoparticles with Tailored Size and Their Application As Unusually Stable and Efficient Propylene Epoxidation Catalyst — ***Nidhi Kapil***, *Fabio Cardinale, Tobias Weissenberger, Panagiotis Trogadas, T. Alexander Nijhuis, Michael Nigra, Marc-Olivier Coppens*

Poster 532dl: Investigating the Sustainability of the Different Types of Catalytic Sites in Aminosilica Materials — ***Jee-Yee Chen***, *Nicholas Brunelli*

Poster 532dm: Single Molecule Studies of the Aldol Condensation of Nile Red Aldehyde with Silica-Bound Acetophenone — *Abdulhafiz Usman, Daniel A. Higgins*, ***Keith Hohn***

Poster 532dn: Flame Stabilized Atomically Dispersed Pd for CO Oxidation — ***Musa Najimu***, ***Erdem Sasmaz***

Poster 532do: Enhancement of Thermal Stability of Binder-Added Mo/HZSM-5 for Methane Dehydroaromatization and Regeneration — ***Ju Nayeong***, *Sang Yun Kim, Kwan-Young Lee*

Poster 532dp: Programmable Catalysts: Metal/Oxide-Graphene Catalytic Condensers — ***Tzia Ming Onn***, *Phillip Christopher, Omar Abdelrahman, Matthew Neurock, K. Andre Mkhoyan, C. Daniel Frisbie, Paul Dauenhauer*

Poster 532dq: Reaction Calorimetry for Adsorption Thermodynamics in Zeolite — ***Ajibola Lawal***, *Omar Abdelrahman*

Poster 532dr: Ti55Cx(x=38,44)@Pt92 Cuboctahedral Core-Shell Nanoclusters for Oxygen Reduction Reaction: A DFT Study — ***Hye Bin Yun***, *Byungchan Han*

Poster 532ds: Mechanistic Study of Hydride Formation over Graphene-Supported Metal Nanostructures — ***Simuck Yuk***, *Walter Cesarski, Tyler Komorowski, Francesca Mangione, Barry-John Baxter, Sebastien Thomas, Alisan Behr, Katherine LaReau, Caspar Yi, Enoch Nagelli*

Poster 532dt: Designing Catalytically Active and Thermally Stable Nanoparticles Via *in-Situ* Exsolution — ***Haotian Yang***, *Jiajie Cen, Alexander Orlov*

Poster 532du: Analysis and Augmentation of Guest-Host Interaction Energy Models As CHA and AEI Zeolite Crystallization Phase Predictors — *Craig Waitt*, ***Xuyao Gao***, *Subramanian Prasad, Ahmad Moini, Anthony DeBellis, Rajamani Gounder, William Schneider*

Poster 532dv: Application of Strong Electrostatic Adsorption Using Formed Alumina Commercial Supports for Pt Catalyst — ***Roozbeh Seifollahy-Astaraee***

Poster 532dw: Co-Precipitation Continuous Synthesis of the Ni-Rh-$Ce_{0.75}Zr_{0.25}O_2$ Catalyst in the Membrane Dispersion Microreactor System for *N*-Dodecane Steam Reforming to Hydrogen — ***Qiangqiang Xue***, *Binhang Yan, Yujun Wang, Guangsheng Luo*

Poster 173a: Effects of Domain Size and Support Composition on the Reactivity and Reducibility of Oxide-Supported Tungsten Oxide Clusters — ***Anukriti Shrestha***, *Konstantin Mamedov, Robert J. Davis, Christopher Paolucci*

Poster 532dx: Dynamic Evolution of Metal Nanoparticles in Bifunctional Systems for Catalytic Chemical Upgrading — ***Laura Paz Herrera***, *James Medlin*

Poster 532el: Synthesis of Highly Porous Polymer Microspheres with Interconnected Open Pores and Their Application As Catalytic Microreactors — ***Hyeonbo Shim***, *Mun Ho Kim*

Poster 532dy: Reactive CFD and NMR: Bringing research areas together for detailed, full-field validation — ***Kevin Kuhlmann***, *Mehrdad Sadeghi, Harm Ridder, Georg R. Pesch, Jorg Thöming*

Poster 532dz: A New Correlation for Pressure Drop through Unbounded Randomly Packed Beds of Spherical Catalyst Particles over the Entire Range of Reynolds Number — ***Anthony Dixon***

Poster 532ea: Clarifying Trust of Machine-Learned Catalyst Predictions with Uncertainty Quantification — ***Cameron Gruich***, *Bryan Goldsmith*

Poster 532eb: Infusing Theory into Deep Learning for Interpretable Stability Prediction of Transition Metal Alloys — ***Yang Huang***, *Shih-Han Wang, Hongliang Xin*

Poster 532ec: Incorporation of Covariance of DFT Energy Ensembles into Gnn Models for the Trustworthy Catalyst Design Method — ***Janghoon Ock***, *Tian Tian, Zachary Ulissi*

Poster 532ed: Theory-Infused Neural Network for Interpretable *D*-Band Moments Prediction — ***Shih-Han Wang***, *Yang Huang, Hemanth Pillai, Luke E. K. Achenie, Hongliang Xin*

Poster 532ee: Accuracy of DFT Functionals: A Benchmarking Study to Understand NO Binding on Pd-CHA — ***Surya Pratap Solanki***, *Bhuiyan Md. Rahman, Taha Salavati-fard, Lars Grabow*

Poster 173x: Active Machine Learning Towards Closed-Loop Optimization for High Throughput Experimentation — ***Alexander Pomberger***

Poster 173z: Automated Kinetic Rate Equation Discovery – a Methodological Framework — ***Miguel Ángel de Carvalho Servia***, *Antonio del Rio Chanona, Dongda Zhang, Klaus Hellgardt, Mimi Hii*

Poster 173ab: On the Performance of Differential Evolution Optimization in Kinetic Parameter Determination of Propene Polymerization through Modeling & Simulation — ***Nikhil Prakash***

Poster 173af: Machine Learning Prediction of Adsorption Energies over Heterogeneous Catalysts — ***Alexander Summers***, *Q. Peter He*

Poster 532ef: Development of Novel Catalyst for Ammonia Oxidative Decomposition — ***Soohang Lee***, *Seok-Ho Lee, Seorin Ji, Kwan-Young Lee*

Poster 532eg: Single-Atom Alloy Pd/Pt in Fe As Catalysts for Electrocatalytic Nitrate Reduction — ***Yuanqi Liu***, *Huiyuan Zhu*

Poster 532el: Parametric Sensitivity Analysis of the Transient Adsorption-Diffusion Models for Hydrocarbon Transport in Microporous Materials — ***Vladyslav Shostak***, *Evgeniy Redekop, Unni Olsbye*

Poster 532eh: Recent Progress on Optimizing Haber-Bosch Ruthenium Catalysts through Multiscale Modelling — ***Blaž Likozar***, *Sašo Gyergyek, Luka Skubic, Janvit Terzan, Anže Prašnikar, Anja Sedminek, Žiga Ponikvar, Matej Huš*

Poster 532ei: Using Ru-Doped TiO_2 Clusters for Photoactivation of N_2 — *Taja Žibert, Blaž Likozar,* ***Matej Huš***

Poster 532ej: Design of a Novel Ru-Based Nrr Catalyst Using a Framework Integrating DFT and Kmc — ***Chi-Ho Lee***, *Silabrata Pahari, Joseph Kwon*

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(533) Poster Session: Environmental Division

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, North Hall E

Alexander Orlov, Chair
Jason Trembly, Co-Chair
Kristina Wagstrom, Co-Chair

Sponsored by: Environmental Division

Poster 533a: Selective Capture and Mineralization of CO_2/SOx Gas Using Industrial Wastewater. — ***Won Yong Choi***, *Yunsung Yoo, Dongwook Lee, Kyu Jang, Jinwon Park*

Poster 533b: Plastic Pyrolysis Gas Purification and Polymorph Control of Metal Carbonate Using Captured CO_2 By Deep Eutectic Solvents — ***Kyumin Jang***, *Won Yong Choi, Dongwook Lee, Yunsung Yoo, Jinwon Park*

Poster 533c: Perstraction: A Membrane-Assisted Liquid-Liquid Extraction Process for Removing Pfas from Water — ***Catherine Almquist***

Poster 533d: A Study on Imidazole-Alkanolamine-Based Deep Eutectic Solvents (DES) Functionalized for Low-Concentration Sulfur Dioxide Absorption — ***Dongwook Lee***, *Yunsung Yoo, Kyu Jang, Won Yong Choi, Jinwon Park*

Poster 533e: Thermo-Responsive Hydrogel with Deep Eutectic Mixture Co-Monomer As Drawing Agent for Forward Osmosis — ***Anelyn Bendoy***, *John Edward Sio, Hana Zeweldi, Hern Kim, Wook-Jin Chung, Grace Nisola*

Poster 533g: Surface Phenomenon Affecting Removal Efficiency of Nitrate from Water on Dispersed Single Atoms in Cu Metal Catalyst: An Ab-Initio Study — ***Srishti Gupta***, *Adam Chismar, Matthew Shaffer, Daniel J. Rivera, Christopher Muhich*

Poster 533h: Bench-Scale Testing of Electrochemical Recovery of Phosphorus from Post-Digester Municipal Wastewater Driven By Magnesium Salt — ***Lawrence Ajayi***, *Sana Heydarian, Jason Trembly, Damilola Daramola*

Poster 533i: A Life Cycle Assessment Study of Wind Power Based Multi- Source Energy Systems — *Joon Heon Lee,* ***Jun Hyung Ryu***

Poster 533j: The Characterization of Corrosion Inhibitors from Quinazolinones and Benzoxazines Derivatives By Electrochemical Methods — ***Muzammil Nishar Ahmed***, *Nishal Egodawaththa, Noel Manring, Nasri Nesnas, Pavithra Pathirathna*

Poster 533k: Understanding Integrated Carbon Negative Systems — ***Elizabeth Abraham***, *Dhabia Al-Mohannadi*

Poster 533l: Magnetic Hierarchical Titanium-Ferrocyanide for the Removal of Radioactive Cs from Water — ***Hee-Man Yang***

Poster 533m: Decrease of Biological Contamination from Municipal Wastewater By Entrapped Nzvi in Cellulose Acetate: Operating Conditions, Reduction Mechanisms with AI Applications — ***Ahmed Mahmoud***, ***Robert Peters***, ***Mohamed Mostafa***

Poster 533n: Remote Monitoring, Supervisory Control and Technoeconomic Evaluation of Advanced High Recovery Wellhead Water Purification and Desalination Systems — ***Yoram Cohen***, *Bilal Khan, Christian Aguilar, Mitchell Rogers, Yang Zhou, Nora Marki*

Poster 533q: Cationic Dye Adsorption on Metal Organic Framework: An Equilibrium Study — ***Saif Mehdi***, *Kannan Aravamudan*

Poster 533r: A Comprehensive Study to Evaluate the Removal Capacity of Heavy Metal Ions and Dissolved Organics from Produced Water Using Vadose Zone Soils for Soil Aquifer Treatment — ***Jisha Ali***, *Tu Pham Le Phuong, Abdulfahim Arangadi, Emad Alhseinat*

Poster 533s: Joining Lab Experiments and CFD-Amozone Model for Deep Understanding of Batch Ozonation and Improve Experimental Method — *Giacomo Bellandi, Roberta Muoio, Min Yang, Kevin Guerrero, Arantxa Sanchez, Andrea Börgers, Ruud Schemen, Peter van Dijk, Pieter Vlasschaert, Usman Rehman, Arne Wieland, Jochen Türk, Wim Audenaert,* ***Ingmar Nopens***

Poster 533t: Application of Waste Materials As Demulsifier for Oil/Water Separation — *Ahmad Adewunmi,* ***Muhammad Shahzad Kamal***, *Shirish Patil, Syed Hussain, Afeez Gbadamosi*

Poster 533u: Hydrogen Production Via Ammonia Decomposition over Ni-Pt/Al_2O_3 using Electrical Heater: A Multi-Objective Optimization — ***Ali Cherif***, *Chul-Jin Lee*

Poster 533v: Economic, Social and Ecological Benefits of Optimization of Agrivoltaic-Biomass Based Renewable Energy System — ***Anubha Agrawal***, *Bhavik Bakshi, Hariprasad Kodamana, Manoj Ramteke*

Poster 533w: Methanotrophic Activity in the Deep Environment: Enhancement of Methane Catalysis Rates — ***Dipayan Samanta***, *Rajesh K. Sani*

Poster 533y: Understanding the Transport and Fate of the Microplastic Particles in a Main Wastewater Treatment Plant: Case Study of a Typical Plant in Western Iran — ***Shafieh Karami***, *Rashed Rashidi, Pedro E. Arce, Negar Saraei*

Poster 629b: Chemical Recycling of Agricultural Waste Plastic By Pyrolysis: Case of Study of Province of Buenos Aires, Argentina — *Gabriel Rodriguez Garrido, Pablo Marinangeli, Maria Alicia Volpe,* ***Patricia Hoch***, ***Maria Soledad Diaz***

Poster 473e: Advanced Oxidative Degradation of Polyethylene for Sustainable Upcycling — ***Shoumik Sadaf***, *Zhihua Jiang*

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(534) Poster Session: Novel Products from Forest and Plant Biomass

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, North Hall E

Xuejun Pan, Chair
Shijie Liu, Co-Chair

Sponsored by: Forest and Plant Bioproducts Division

Poster 534b: Application of Protocatechuic Acid-Based Deep Eutectic Solvent for Utiliztion of Engineered Biomass — *Yunxuan Wang,* ***Anqi Ji***, *Xianzhi Meng, Yang Tian, Linjing Jia, Aymerick Eudes, Kwang Ho Kim, Yunqiao Pu, Gyu Leem, Deepak Kumar, Jeong Jae Wie, Arthur Ragauskas, Chang Geun Yoo*

Poster 534c: Effects of pH and Multistage ALPHA Process on the Phase Behavior of Kraft Lignin — ***Oreoluwa Agede***, *Graham W. Tindall, Mark C. Thies*

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(535) Poster Session: Fuels and Petrochemicals Division

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, North Hall E

Paul Mathias, Chair

Sponsored by: Fuels and Petrochemicals Division

Poster 535a: Acetylene Powered Thermal Power Plant Boiler — ***Debshilpi Patra***

Poster 535b: A Novel Fluid System to Integrate Stimulation, EOR, and CO2 Storage in Shale Oil Reservoirs — ***Yang Zhao***, *Yanxu Ding*

Poster 535c: Fluoro- Vs Hydrocarbon Surfactants: Synthesis and Application in Enhanced Oil Recovery — ***Syed Hussain***, *Muhammad Shahzad Kamal, Ahmad Mahboob, Mobeen Murtaza, Shirish Patil, Emad W. Al Shalabi*

Poster 535d: Fast Pyrolysis of Food Waste in N_2 and CO_2 after Torrefacton in a Bubbling Fluidized Bed Reactor — ***Seung-Soo Kim***, *Hoang Vu Ly, Jinsoo Kim, Hyun Tae Hwang*

Poster 535e: Thermogravimetric and Kinetic Study of *Hemp* and *Milkweed* — ***Seung-Soo Kim***, *Jinsoo Kim, Foster Agblevor*

Poster 535f: pH and Salt-Responsive Dynamic Binary Complexes Based on Supramolecular Complexation with Applications in Unconventional Reservoirs — ***Bhargavi Bhat***, *Shuhao Liu, Yu-Ting Lin, Joseph Kwon, Mustafa Akbulut*

Poster 535g: Upgrading Tire-Derived Pyrolysis Oil Via Distillation for Blending with Fuel Oils — *Ryan Dantu, Johannes Knoetze,* ***Cara Schwarz***

Poster 535h: Development of Bioethanol from Molasses: A Modern Approach — ***Ayush Gondane***, *Tanashree Paraye, Dr. Utkarsh Maheshwari*

Poster 535i: Crude Assays Cut Properties — ***Andrew Sloley***

Poster 535j: Screening Criteria and Experimental Investigation for Enhanced Oil Recovery at Umm Niqa Oil Field-Kuwait — *Ahmed AlShammri, Osamah Alomair,* ***Adel Elsharkawy***

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(536) Poster Session: Particle Technology Forum

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, North Hall E

Michael Molnar, Chair

Sponsored by: Particle Technology Forum

CHARACTERIZATION AND STRUCTURE OF SOLID MATERIALS

Poster 536a: A Revolutionary, Evolutionary Approach to Particle Characterisation — ***Kit Windows-Yule***

Poster 536c: Effects of Particle Size, Shape and Moisture Content on the Flowability of Microcrystalline Cellulose Powder — ***Jordan Monroe***, *Heather Emady*

PROCESSING METHODS

Poster 536d: A Comparative Evaluation of Ca-Based Wastes for a Oxy-Fuel Circulating Fluidized Bed Combustor — ***See Hoon Lee***, *Hyun Jun Park, Chul Seung Jung, Jung Min Sohn, Sang Mun Jeong*

Poster 536f: Scale-up of Drying of Supported Catalysts in a Fluidized Bed — ***Carlin Leung***, *Justin Adler, Tim A. G. Langrish, Benjamin Glasser*

Poster 536h: Conduction and Radiation Heat Transfer in a Rotary Drum — ***Bhaumik Bheda***, *Heather Emady*

Poster 536p: Optimization of Low Dose Powder Filling Process for Dry Powder Inhalers — ***Tanu Mehta***, *Zhanjie Liu, Bruhal Shah, Justin P. Lacombe, Bodhisattwa Chaudhuri*

ENGINEERED PARTICLES

Poster 536j: Magnetic Hyperthermia in Biosimilar Colonic Tumor Environment Using Silica-Coated Superparamagnetic Iron Oxide Nanoparticles — ***Yuming Zhang***, *Alexandra Teleki*

Poster 536k: Bioactivity of Flame-Made Calcium Phosphate Bionanomaterials for Bone Tissue Engineering — ***Yael del Carmen Suárez López***, *Georgios Sotiriou*

Poster 536l: Manufacture of Complex-Shaped Tungsten Materials Via Atomic Layer Deposition and Direct Ink Writing — ***Hailey Loehde-Woolard***, *Elena Napoletano, Davis R. Conklin, Bergen Evans, James Smay, Alan Weimer*

Poster 536m: Exploring $LaFeO_3$ oxygen Carriers for Reactivity Enhancement through Structural Changes in Chemical Looping Partial Oxidation System — ***Anuj Joshi***, *Sonu Kumar, Lang Qin, Zhuo Cheng, Hendrik Colijn, Zain Mohammad, Liang-Shih Fan*

Poster 536n: Refractory Tungsten ALD Coatings for Nuclear Thermal Propulsion Fuel Elements — ***Davis R. Conklin***, *Sarah Bull, Christopher G. McKinney, Jamelle K.P. Williams, Arne Croell, Jhonathan Rosales, Alan Weimer*

Poster 536o: Designing Targeted Magnetic Nanoparticles Via Click Chemistry to Diagnose Inflammatory Bowel Disease — ***Shno Asad***, *Christel A.S. Bergström, Alexandra Teleki*

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(537) Poster Session: Process Development

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, North Hall E

Vinod Kumar Venkatakrishnan, Chair

Sponsored by: Process Development Division

BLUE AMMONIA

Poster 537a: Energy, Economic and Environmental (3E) Analysis and Multi-Objective Optimization of Natural Gas Based Blue Ammonia Process — ***BeomJu Shin***, *Jong-Ho Moon*

Poster 537b: 3E (Energy, Economic and Environmental) Analysis for Natural Gas Based Blue Ammonia Synthesis Process through Multi-Objective Optimization — ***BeomJu Shin***, *Mun Jihun, Jong-Ho Moon*

DISTILLATION

Poster 537c: Process Intensification of a Complex Ternary Azeotropic Distillation System Via Structural Variations — *Chaeyeong Seo, Heecheon Lee,* ***Minyong Lee***, *Jae Lee*

Poster 537d: Temperature Driven Internal Heat Integration for Designing a Novel Energy-Efficient Double Annular Reactive Distillation Column — *Chaeyeong Seo, Heecheon Lee,* ***Minyong Lee***, *Jae Lee*

PROCESS MODELLING

Poster 537e: Production of Ethanol and Acetic Acid from Syngas Via Carbonylation of Dimethyl Ether: Kinetic and Process Modeling — ***Seungwoo Kim***, *Hyun Seung Jung, Won Bo Lee, Myung-June Park, Jong Wook Bae*

PHARMACEUTICAL MANUFACTURING

Poster 537f: Resilient Multi-Site Onboarding, Knowledge Transfer and Process Understanding of Commercial Drug Substance Manufacturing: Virtual Make-a-Batch Exercise — ***Muhammad Irfan***

Poster 537i: Development and Demonstration of an Ultra-High Temperature Continuous Racemization Process — ***Ali Hasan***, *Kiersten Campbell, Jillian Sheeran, Kevin Nagy, David D. Ford, Yuan-Qing Fang*

CAREER DEVELOPMENT

Poster 537g: Building an Exciting Career Supporting the Energy Transition Journey — ***Vinod Kumar Venkatakrishnan***, *Juben Chheda*

Poster 537h: Photocatalytic Process Optimization for Toxic Gases Removal: Mass Transfer Effect Elimination Efficiency of Chemical Weapon Agent (Simulant) — ***Youcef Serhane***, *Abdelkrim Bouzaza, Dominique Wolbert, Aymen Amin Assadi*

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(538) Poster Session: Sustainability and Sustainable Biorefineries

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, North Hall E

Clayton Jeffryes, Chair
Ashley Pennington, Co-Chair

Sponsored by: Sustainable Biorefineries

CARBON DIOXIDE ENGINEERING

Poster 538a: Oxidative Coupling of Methane with CO2 Using Sr/La2O3 and the Effect of Oxygen Addition — ***Hyewon Lee***, *William Northrop*

Poster 538b: Role of Ba in Low-Temperature Thermochemical Conversion of Carbon Dioxide with $LaFeO_3$ Perovskite Oxides — *Hanzhong Shi, Venkat Bhethanabotla,* ***John Kuhn***

Poster 538c: Optimizing Pore Space Utilization with Foam for Carbon Storage in Powder River Basin Near the Dry Fork Station — ***Ying Yu***, *Davin Bagdonas, Charles Nye, Zunsheng Jiao, Jonathan 'Fred' McLaughlin, Scott Quillinan*

Poster 538d: Evaluation of Novel CO2 Capture Process Configurations with Combined Cycle Gas Turbine Plants — ***Mohammad Nahyan Arshad***, *Ahmed Al Hajaj*

Poster 538f: Optimization of Amines-CO2 Capture Based on the Absorption-Desorption Process Considering Multiple Objectives — ***Ilse María Hernández-Romero***, *Fabricio Nápoles-Rivera, Antonio Flores-Tlacuahuac*

Poster 538v: Study on Catalytic Carbonylation of Glycerol with CO_2 in Mild Condition over Cerium Oxide/Zinc Oxide Catalysts — *Soon Long Low,* ***Bing-Hung Chen***

Poster 538u: Current Technology Development for CO2 Utilization into Synthetic Fuels: Challenges and Opportunities — ***Bachirou Guene Lougou***, *Yong Shuai*

BIO-ENVIRONMENTAL ENGINEERING

Poster 538g: Novel Strategies with Artificial Floating Islands for Water Bodies Restoration As Optimal Control Problems — *Laura Fritz, Amira Siniscalchi, Vanina Estrada,* ***Maria Diaz***

Poster 538h: Using the γ-Valerolactone Biorefinery to Fractionate Biomass into Sugar and Phenolic Streams for Microbial Conversion to Fuels and Co-Products — ***Steven Karlen***, *Jason Coplien, Canan Sener, Yaoping Zhang, Miguel Perez, German Umana, Timothy J. Donohue, John Ralph, Daniel R. Noguera*

Poster 538j: Recycling of Plastic Waste Using Dissolution/Precipitation — ***Christian Ferger***, *Paschalis Alexandridis, Marina Tsianou*

Poster 538k: Post-Consumer PET Chemical Recycling into Monomers for the Circular Economy — ***Richard-Joseph Peterson***

Poster 538l: Recycling of Plastic Wastes By Solvent-Targeted Recovery and Precipitation — ***Jiuling Yu***, *Kevin Sanchez-Rivera, Panzheng Zhou, Aurora del Carmen Munguía-López, Jiaze Ma, Zhuo Xu, Victor Sanfins Cecon, Kevin Nelson, Greg W. Curtzwiler, Keith Vorst, Ezra Bar Ziv, Victor M. Zavala, Reid Van Lehn, George Huber*

Poster 538m: Social and Environmental Assessments of Tourism: A Case-Study — *Jan Puhar, Uroš Novak, Lidija Čuček,* ***Annamaria Vujanović***

CHEMICAL-ENVIRONMENTAL ENGINEERING

Poster 538o: Methanolysis of PET As a Model Chemical Recycling Method for Heterochain Polymers — ***Hannah Pineault***, *Nicholas Brunelli*

Poster 538p: Co-Generation of Hydrogen and High-Value Carbon from Methane in a Gas-Solid Fluidized-Bed Reactor — ***Woohyun Kim***, *Kang Seok Go, Byungwook Hwang, Daewook Kim, Keon Bae, Dung A. Pham, Seon Joo Park, Se-eun Jung, Ji Sun Im*

Poster 538q: The Olefin-Intermediate Process (OIP): A Means to Depolymerize & Upcycle Waste Plastics — ***Lucas Ellis***, *Kevin Sullivan, Nicholas A. Rorrer, Yuriy Roman, Gregg T. Beckham*

Poster 538r: Development of Biodegradable Plastic Material from Lignin and Depolymerized Synthetic Plastic Copolymer — ***David Chem***, *Keisha Walters*

Poster 538s: Waste Management in Bio-Diesel Production — ***Vedant Telrandhe***, *Dr. Utkarsh Maheshwari*

Poster 538t: Hydrogen Release Kinetics of Thermal Hydrolysis of Sodium Borohydride and Hydrate — ***Savannah G. Hunt***, *Hyun Tae Hwang*

Poster 538w: New Era of Carbon Capture and Utilization Technology with Reaction Swing Absorption — *Kezia Megagita Gerby Langie, Kyungjae Tak, Dahye Won,* ***Ung Lee***

Poster 538x: Production of Neo Acids from Biomass Waste — ***Erha Andini***, *Sunitha Sadula, Dionisios Vlachos*

Poster 538y: Electrochemical Conversion of Waste Nitrate to Hydroxylamine — ***Manish Mosalpuri***

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(539) Poster Session: Waste Plastics

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, North Hall E

Jeffrey Seay, Chair

Sponsored by: Waste Plastics

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(540) Poster Session: Transport and Energy Processes Division

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, North Hall E

Gus Georgeton, Chair

Sponsored by: Transport and Energy Processes

Poster 540a: Hybrid Approach for Accelerating the Implementation of Hydrogen Infrastructure Using Experience Based Data Formatting and Systematic Decision-Making Framework — *Soo Hwan Kim,* ***Jun-Hyung Ryu***

Poster 540b: Supercapacitors Based on Graphene Quantum Dots for Efficient Energy Storage — *Ayse Saliha Korkut,* ***Betul Uralcan***

Poster 540c: Optimization of Energy Density in Supercapacitors By Utilizing a Hybrid Artificial Neural Networks-Genetic Algorithm Based Optimization Algorithm — *Duygu Kaya,* ***Betul Uralcan***

Poster 540d: Tuning Gas Diffusion Electrode Construction to Mitigate Flooding and Degradation Processes for Electrochemical CO2 Reduction — ***Khantey Lim***, *Xiao Kun Lu, Bingzhang Lu, Linsey Seitz*

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(541) Plenary Session: Computational Molecular Science and Engineering Forum (Invited Talks)

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, N-224AB

Sapna Sarupria, Chair
Jim Pfaendtner, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

3:30 Paper 541a: Understanding and Controlling Properties of Biomimetic Polymers — ***Jim Pfaendtner***

4:10 Paper 541b: The Influence of Halides on the Solution-Phase Growth of Cu Nanowires and Microplates: A Multi-Scale Theoretical Study — ***Kristen Fichthorn***

4:30 Paper 541c: Mechanochemical Activation in Nanostructured Triblock Copolymers: A Computational Study — ***Antonia Statt***

5:10 Paper 541d: Modeling the Recycling of Polymer Waste — ***Sanat K. Kumar***

5:30 Paper 541e: How Molecular Simulations Are Being Used to Phase out High Global Warming Potential Hydrofluorocarbon Refrigerants — ***Edward Maginn***

(542) Advances in Computational Methods and Numerical Analysis - II

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, W-101C

Joel Paulson, Chair
Wheaton Schroeder, Co-Chair
Matthew Stuber, Co-Chair

Sponsored by: Applied Mathematics and Numerical Analysis

3:30 Paper 542a: Surrogate Modeling of 3D Flow Dynamics and Chemical Reactions Using Physics-Constrained Deep Learning — ***Youngseok Bak**, Jong Min Lee*

3:49 Paper 542b: A Machine Learning Approach to Bridge the Gap between the Kuramoto-Sivashinsky and the Navier-Stokes Equations for Thin Film Flow — ***Cristina Martin Linares**, Eleni Koronaki, Georgios Psarellis, George Karapetsas, Ioannis G. Kevrekidis*

4:08 Paper 542c: A Data-Driven Approach to Determining Problem Well-Posedness — *Thomas Bertalan, Elizaveta Rebrova, George Kevrekidis, **Ioannis G. Kevrekidis***

4:27 Paper 542d: Nonlinear Data Fusion from Heterogeneous Partial Observation Sets — ***David Sroczynski**, Erez Peterfruend, Ronald Coifman, Ioannis G. Kevrekidis*

4:46 Paper 542e: Learning What to Learn: Common and Sensor-Specific Information across Multiple Sensors, with Some Thoughts about Sensor Spoofing and Causality — ***David Sroczynski**, Felix Dietrich, George Kevrekidis, Ronen Talmon, Matthew Williams, David Siu, Ioannis G. Kevrekidis*

5:05 Paper 542f: Towards Exact Designs in Optimal Experiment Campaigns — ***Marco Sandrin**, Benoit Chachuat, Constantinos C. Pantelides*

5:24 Paper 542g: Squeeze Functional Approach for Adaptive Step Size in Solving Stiff ODE/Dae Problems — ***Gang Xu**, Mark Stadtherr*

5:43 Paper 542h: Partial Multiparametric Programming for Accelerating Optimal Control, Applied to an Air Separation Unit — ***Dustin Kenefake**, Efstratios N. Pistikopoulos*

(543) Advances in Machine Learning and Intelligent Systems II

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, W-102A

Qi Zhang, Chair
Seongmin Heo, Co-Chair

Sponsored by: Information Management and Intelligent Systems

3:30 Paper 543a: A Multi-Fidelity, Physics-Informed Approach to Active Learning-Guided Experiment Design for the Study of Ammonia Synthesis Via Plasma Catalysis — ***Ketong Shao**, Ali Mesbah*

3:49 Paper 543b: A Data Reconciliation Methodology for Reduced Order Modeling of Process Systems — ***Arijit Chakraborty**, Harshal Marathe, Venkat Venkatasubramanian*

4:08 Paper 543c: Improved Long-Short Term Memory Model for Dynamic and Multimodal Processes Based on K-Means Clustering: Application to an Industrial 2, 3-Bdo Distillation Process — ***Yeongryeol Choi**, Bhavana Bhadriraju, Hyungtae Cho, Jongkoo Lim, Il Moon, Joseph Kwon, Junghwan Kim*

4:27 Paper 543d: Computer-Aided Fuel Design with Generative Graph Machine Learning — ***Jan G. Rittig**, Martin Ritzert, Artur M. Schweidtmann, Stefanie Winkler, Jana M. Weber, Philipp Morsch, Karl A. Heufer, Martin Grohe, Alexander Mitsos, Manuel Dahmen*

4:46 Paper 543e: Simultaneous Hybrid Modeling of Distillation Towers with a Linear Correction Model for Different Tower Operations — ***Carlos Rodriguez**, Prashant Mhaskar, Vladimir Mahalec*

5:05 Paper 543f: Offset-Free Deep Deterministic Policy Gradient with Lyapunov Learning Penalties — ***Elijah Hedrick**, Katherine Hedrick, Debangsu Bhattacharyya, Stephen Zitney, Benjamin P. Omell*

5:24 Paper 543g: Premexotac: Bitterants *in-Silico* Screening Using Machine Learning for Advanced Pharmaceutical Development — ***Gerardo De León**, Eleonore Fröhlich, Sharareh Salar-Behzadi*

5:43 Paper 543h: On-Line Learning in Model Predictive Control of Nonlinear Processes: Generalization Guarantees and Stability Analysis — *Cheng Hu, **Zhe Wu***

(544) Integrated Product and Process Design

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, W-101A

Davood Babaei Pourkargar, Chair
Matthew Stuber, Co-Chair

Sponsored by: Systems and Process Design

3:30 Paper 544a: Combining Solvent Screening with Process Synthesis for Separating Refrigerant Mixtures Using Ionic Liquids — ***Mohammed Sadaf Monjur**, Ashfaq Iftakher, M M Faruque Hasan*

3:51 Paper 544c: Computer-Aided Molecular and Process Design: Optimal Solvent Design for CO_2 Chemical Absorption Processes Using SAFT-γ-Mie Equation of State — ***Ye Seol Lee**, **Claire Adjiman**, Amparo Galindo, George Jackson*

4:12 Paper 544d: Optimization of a Flexible Carbon Capture-Equipped Power Plant Integrated with Lime-Based Direct Air Capture Under Time-Varying Electricity Prices — ***Edward Graham**, Moataz Sheha, Dharik Mallapragada, Emre Gençer, Howard Herzog, Phillip Cross, James Custer, Adam Goff, Ian Cormier*

4:33 Paper 544e: Optimization-Based Design of Renewable Methanol Production Encompassing Waste Heat Utilization with the Fluxmax Approach — ***Tibor Svitnic**, Kai Sundmacher*

4:54: Break

5:15 Paper 544g: Incorporating Materials Surrogate Models into Process Models for Adsorption-Based Gas Seperations — ***Xiangyu Yin**, Lorenz T. Biegler, Chrysanthos Gounaris*

(545) Networked, Decentralized, and Distributed Control

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, W-101B

Helen Durand, Chair
Wentao Tang, Co-Chair

Sponsored by: Systems and Process Control

3:30 Paper 545a: Near-Optimal Distributed Linear-Quadratic Regulator for Networked Systems — ***Sungho Shin**, Yiheng Lin, Guannan Qu, Adam Wierman, Mihai Anitescu*

3:49 Paper 545b: On the Emergence of Symmetric Problem Structure in the Model Predictive Control of Numbered-up Modular Facilities — ***Yi Dai**, Andrew Allman*

4:08 Paper 545c: Improving Computational Efficiency of Machine Learning-Based Distributed Predictive Control of Nonlinear Processes Using Feature Selection — *Tianyi Zhao, Yingzhe Zheng, Cheng Hu, **Zhe Wu***

4:27 Paper 545d: Encrypted Model Predictive Control Design for Security to Cyber-Attacks — ***Atharva Vijay Suryavanshi**, Aisha Alnajdi, Zhe Wu, Panagiotis Christofides*

4:46 Paper 545e: From Statistical Mechanics to Distributed Process Control — ***Erik Ydstie***

5:05 Paper 545f: Optimal Resource Allocation in a Subsea Oil Production Network Using Distributed Feedback-Optimizing Control Based on Primal Decomposition — ***Risvan Dirza**, Sigurd Skogestad, Dinesh Krishnamoorthy*

5:24 Paper 545g: Distributed and Multiple Model Predictive Control for Rapid Load-Following Operation of Supercritical Pulverized Coal Power Plants — ***Sung Min Choi Hong***, *Elijah Hedrick, Katherine Hedrick, Daniel Beahr, Debangsu Bhattacharyya, Stephen Zitney, Benjamin P. Omell*

5:43 Paper 545h: Dynamic Analysis and Stabilization of a Packed Bed Reactor (PBR) — ***Guilherme Ozorio Cassol Sr.***, *Stevan Dubljevic*

(546) Education Division Awards Plenary (Invited Talks)

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, W-105B

Daniel Lepek, Chair
Benjamin Davis, Co-Chair

Sponsored by: Undergraduate Education

3:30: Welcoming Remarks

3:35 Paper 546a: Innovating Real World Global Challenges in Chemical Engineering Education — ***Courtney Pfluger***

4:05 Paper 546b: Professional Service: A Rewarding & Cautionary Tale — ***Anthony Butterfield***

4:35 Paper 546c: Envisioning the Future of Chemical Engineering Education — ***Cheryl A. Bodnar***

(547) Survey Results and Best Practices (Invited Talks)

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, W-105A

Laura Ford, Chair

Sponsored by: Undergraduate Education

3:30 Paper 547a: Capstone Design with Practical Characteristics for a New Era — ***Gavin Towler***

4:00 Paper 547b: How We Teach: Capstone Design Survey Results — ***Laura Ford***, *Janie Brennan, Jennifer Cole, Marnie Jamieson, Kevin Dahm, David Silverstein, Troy Vogel*

4:30 Paper 547c: How We Teach: Capstone Design Discussion — ***Laura Ford***

(548) Overcoming the Bystander Effect in Chemical Engineering Ethics

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, N-231B

Sindia M. Rivera-Jimenez, Chair
Shannon Servoss, Co-Chair

Sponsored by: The Role of Intersectionality in Chemical Engineering

(549) Lithium & Beyond: Fundamental Advances in High Performance Batteries II

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, N-231A

Alexander Urban, Chair
Nian Liu, Co-Chair
Vilas G. Pol, Co-Chair
Theresa Schoetz, Co-Chair

Sponsored by: Electrochemical Fundamentals

3:30 Paper 549a: Driving Force behind the Amorphization in the Crystalline Cathode Structures during Alkali Metal Ion Intercalation for Electrochemical Energy Storage — ***Omer Ozgur Capraz***, *Bertan Ozdogru*

3:50 Paper 549b: Impact of Dopant Oxidation State on the Stability of Ni-Rich Layered Cathode Materials for Durable Li-Ion Batteries — ***H. Hohyun Sun***, *Un-Hyuck Kim, Adam Heller, Chong Seung Yoon, C. Buddie Mullins*

4:10 Paper 549c: Understanding the Cation-Mixing Mechanism in Ni-Rich Cathodes from First Principles — ***Cem Komurcuoglu***, *Yunhao Xiao, Xinhao Li, Zheng Li, Alan West, Alexander Urban*

4:25 Paper 549d: Molecular mobility in hybrid solid-liquid lithium ion electrolytes studied with diffusion NMR — ***Martina Cattaruzza***, *Yuan Fang, István Furó, Göran Lindbergh, Mats Johansson*

4:40 Paper 549e: Deeply Rechargeable Zinc Anodes for High-Energy Aqueous Batteries — ***Nian Liu***

5:00 Paper 549f: Investigation of Calcium Zincate ($CaZn_2(OH)_6 \cdot 2H_2O$) Anodes for Rechargeable Alkaline Zinc Nickel Batteries — ***Patrick Yang***, *Damon E. Turney, Stephen O'Brien, Sanjoy Banerjee*

5:15 Paper 549g: Ternary Ionic Liquid Analogues for Rechargeable Metal Aluminum Batteries — ***Jonah Wang***, *Theresa Schoetz, Elizabeth Biddinger, Robert Messinger*

5:30 Paper 549h: Rechargeable Al-CO_2 Battery Enabled By a Homogeneous Redox Mediator with Ultra-Low Overpotential — ***Christopher Fetrow***, *Cameron Carugati, Shuya Wei*

(550) Microfluidic and Microscale Flows: Separations and Particulates

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, N-231C

Travis Walker, Co-Chair
Vivek Narsimhan, Co-Chair

Sponsored by: Fluid Mechanics

3:30 Paper 550a: Computer Recognition of Bacteria in Blood Plasma and Placement in Droplets for Antimicrobial Testing — ***Chandler A. Warr***, *Parker Johns, Katie Holland Ebert, Gregory P. Nordin, William Pitt*

3:45 Paper 550b: Investigation of Novel Core-Shell Microparticles with Degradable Shells for Controlled-Delivery Applications — *Whytneigh Duffie*, ***Travis W. Walker***

4:00 Paper 550c: Separation of Binary Rigid and Deformable Particles with Varying Moduli in Microfluidic Flow — ***Sabrina Marnoto***, *Sara Hashmi*

4:15 Paper 550d: Buckling and Transport of Heterogeneously Stiff Elastic Fibers in Microscale Flows — ***Thomas Minh Nguyen***, *Harishankar Manikantan*

4:30: Break

4:45 Paper 550f: Surface Discretization Considerations for the Boundary-Element Method Applied to Ellipsoidal Particles in Stokes Flow — ***Vivek Narsimhan***, *Charlie Lin, Shiyan Wang, Sangtae Kim*

5:00 Paper 550g: Diffusiophroesis-Controlled Separation of a Colloid-Electrolyte Suspension Under Gravity and Solvent Evaporation — ***Henry Chu***, *Jinjie Xu, Zhikui Wang*

5:15 Paper 550h: Fundamentals of the Fluid Particle Dynamics Method for Simulating the Chemohydrodynamics of Passive and Active Colloids — ***Douglas Tree***, *Qinyu Zhu, Rami Alhasan*

5:30 Paper 550i: Simultaneous Characterization of Thermophoresis and Fluid Properties Using Multiple Particle Tracking Microrheology — ***Maria Chiara Roffin***, *Nazrin Hasanova, Kelly Schultz, James Gilchrist*

(551) Modeling of Interfacial Systems

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, N-232C

Patricia Taboada-Serrano, Chair
Manuela Ayee-Leong, Co-Chair

Sponsored by: Interfacial Phenomena

3:30 Paper 551a: Molecular Simulations of Zeolitic Nanotubes in Aqueous Environments — ***Kevin Hinkle***

3:45 Paper 551b: Computational and Experimental Studies on Amended Montmorillonite Clays for the Adsorption and Detoxification of Benzene — ***Phanourios Tamamis***, *Kendall Lilly, Kelly J. Rivenbark, Meichen Wang, Timothy D. Phillips*

4:00 Paper 551c: Adsorption of Surfactants on Gold Nanoparticles Studied Via Molecular Simulations — ***Abolfazl Faeli Qadikolae***

4:15 Paper 551d: Molecular Interactions at Calcite-Aerosol OT Interface As a Model for Surfactant Mediated Mineralization — *Anuradha Bhat, Tej Choksi, Michael T. Harris*, ***Vance Jaeger***

4:30 Paper 551e: Modeling Surface Tension Using Gibbs'-Tolman Approach — ***Madhavan D.K. Nampoothiri***, ***Sasidhar Gumma***

4:45 Paper 551f: *Surface Tensions of Organophosphorus Compounds.* — ***Ella Ivanova****, Ashvinkumar Vasudevan, Elif Irem Senyurt, Mirko Schoenitz, Alexei Khalizov, Edward L. Dreizin, Gennady Gor*

5:00 Paper 551g: Phase Separation in Metastable and Unstable Regime Effect of Nucleation — ***Abhishek Kumar Barnwal***

5:15 Paper 551h: Evaporation Driven Instability in Tear Film — *Rajesh Khanna,* ***Shalaka Bhargava***

5:30: Break

5:45 Paper 551j: A Coupled Computational Fluid Dynamic/Population Balance Method to Understand Microstructure in Foams and Emulsions — ***Helen Cleaves****, Weston Ortiz, Christine Cardinal Roberts, Cameron Ahmad, Rekha Rao*

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(552) Solid-Liquid Interfaces

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, N-232B

Stephen Martin, Chair
Sepideh Razavi, Co-Chair
Younjin Min, Co-Chair

Sponsored by: Interfacial Phenomena

3:30 Paper 552a: Cooperative Hydrogen Bonding in Underwater Adhesion — *Zachary Lamberty,* ***Joelle Frechette***

3:45 Paper 552b: Texturing Freezing Droplets — ***Shankar Kharal, Jean-Francois Louf***

4:00: Break

4:15 Paper 552d: Thermodynamic Properties of Antifouling Polyproline II Helix Peptide Monolayers on Gold — ***Rebecca Ahn****, Julie N. Renner*

4:30: Break

4:45 Paper 552f: Hydrophobic/Oleophilic Self-Assembly Monolayers (SAMs) Coating for Oil/Water Separation — ***Aigerim Baimoldina****, Lei Li, Yihan Song, Fan Yang, Goran Jovanovic, Matthew Coblyn*

5:00 Paper 552g: A Hydrophilic/Oleophobic Perfluoropolyether Coating for More Efficient Microchannel-Based Oil-Water Separation — ***Yihan Song****, Fan Yang, Lucas Freiberg, Jad Touma, Michaela Dunleavy, Trevor Sargent, Matthew Coblyn, Cliff Kowall, Goran Jovanovic, Lei Li*

5:15 Paper 552h: Evaluating the Impact of Carbon Microspheres on the Stribeck Curve of Aqueous Lubricant — ***Samuel Solomon****, Noshir Pesika*

5:30 Paper 552i: A Nanometer-Thick Ionic Liquid As Media Lubricant in Hard Disk Drives — ***Alan Tirado***

5:45 Paper 552j: Investigation on Competition at Confined Interfaces: The Interplay between Polymers and Ions for a Binding Site. — ***Pierluigi Bilotto****, Laura Mears, Markus Valtiner*

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(553) Advances in Metabolic Engineering- Eukaryotic Organisms

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, N-125A

Sijin Li, Chair
Dongming Xie, Co-Chair

Sponsored by: Bioengineering

3:30 Paper 553a: Complete Biosynthesis of Diverse Plant-Derived Styrylpyrones in *Saccharomyces Cerevisiae* — ***Yinan Wu****, Maple Chen, Sijin Li*

3:48 Paper 553b: Optimizing Campesterol-Producing Yeast Strains for Enhanced Functional Reconstitution of Plant Membrane Enzyme — ***Shanhui Xu****, Yanran Li*

4:06 Paper 553c: Metabolic and Epigenetic Engineering Enables Temporal Control of Taxane Metabolism in *Taxus Chinensis* Plant Cell Culture — ***Cassandra Brzycki Newton****, Alexandra Harrison, Lauren Revene, Jay Gandhi, Sean Horton, Eric Young, Susan Roberts*

4:24 Paper 553d: Engineering Nucleotide Sugar Metabolism in *S. Cerevisiae* for the Glycosylation of Complex Natural Products and Heterologous Proteins — ***Samantha Crowe****, Yuzhong Liu, Fei Gan, Jay Keasling*

4:42 Paper 553e: Microbial Conversion of Vegetable Oils into Omega-3 Oils — ***Jiansong Qin****, Na Liu, Ya-Hue V. Soong, Elif Kurt, Ashley Willan, Qiuyan Chen, Dongming Xie*

5:00 Paper 553f: Pathway Localization and Redox Engineering of Yarrowia Lipolytica for Fatty Alcohol Production — ***Siva Somasundarama****, Michael Spagnuolo, Mark Blenner*

5:18 Paper 553g: The Future Is Fungi: New Platforms Enable Cell Factories & Interkingdom Devices — ***Eric Young***

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(554) Biotechnological Production of Food and Feed Ingredients

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, N-126B

Hesham El Enshasy, Chair
Ryan Summers, Co-Chair
Shang-Tian Yang, Co-Chair

Sponsored by: Food

3:30 Paper 554b: Engineering of Cyanobacterial Rubisco for Sustainable Production of Essential Amino Acids — ***Muhammad Faisal****, Aditya Sarnaik, Apurv Mhatre, Muhammad Javaid Asad, Ryan Davis, Arul Mozhy Varman*

3:48 Paper 554c: Engineering *Aureobasidium Pullulans* to Overexpress Malate Dehydrogenase in the Reductive Tricarboxylic Acid Pathway for Poly (L-malic acid) Production from Glucose — ***Zhen Qin****, Jun Feng, Shang-Tian Yang*

4:06 Paper 554d: Acetic Acid Production from Glucose and Formate By the Co-Culture of *Clostridium Formicoaceticum* and *Lactobacillus Lactis* — ***Rocky Thapaliya****, Opeyemi Bello, Jie Dong*

4:24 Paper 554e: From Screening to a Scalable System: Investigating the Impact of a Peptide Additive on Struvite Formation and Morphology — ***Jacob Hostert****, Olivia Kamlet, Quincy Spitzer, Paola Giammattei, Zihang Su, Naomi Kane, Julie N. Renner*

4:42 Paper 554f: Recent Advances in Utilization of Fermented Plant Proteins and Their Resulting Hydrolysate and Peptide Fractions for Their *In Vivo* and *in Vitro* Antidiabetic Effects. — ***Bababode Kehinde****, Poorva Sharma*

5:00 Paper 554g: [Keynote] Strain and Bioprocess Engineering to Enhance and Investigate Carbon Efficient Biochemical Production — ***David Nielsen***

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(555) Micro- and Nano-Scale Technologies in Life Sciences I

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, N-126A

Whitney Stoppel, Chair
Christina Bailey-Hytholt, Co-Chair
Bomyi Lim, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

3:30 Paper 555a: Polysalicylic Acid Polymer Microparticle Decoys Therapeutically Treat Acute Respiratory Distress Syndrome — ***Emma Brannon****, William J. Kelley, Michael W. Newstead, Alison Banka, Kathryn E. Uhrich, Colleen E. O'Connor, Theodore J. Standiford, Omolola Eniola-Adefeso*

3:48: Break

4:06 Paper 555c: Fabrication and Characterization of Composite Particles for Controlled Release Drug Delivery Applications — ***Michael L. Felder****, Daniel Kupor, Hanieh Safari, Omolola Eniola-Adefeso*

4:24 Paper 555d: Silk Fibroin Nano- and Micro- Particles As a Potential System for a Novel Hemoglobin-Based Oxygen Carrier (HBOC) — ***Marisa Pacheco****, Jostin Armada, Marina P Fernandez-Campa, Jack W. McNamara, Michael O'Brien, Nickolas A. Davies, Bruce D. Spiess, Whitney Stoppel*

4:42 Paper 555e: Hemoglobin Encapsulated Metal Organic Framework Nanoparticles As an Oxygen Therapeutic with Ultrahigh Encapsulation Efficiency — ***Xiangming Gu**, Andre Palmer*

5:00 Paper 555f: Peptide Amphiphile Micelles As a Biomaterials Platform for Universal Influenza Vaccination — ***Megan Schulte**, Ava Steele, Mariam Morafa, Paul Anderson, Rachel Olson, Bret Ulery*

5:18 Paper 555g: Invited Talk: Placeholder for Micro and Nano Scale Technologies I — ***Whitney Stoppel**, Bomyi Lim, Christina Bailey-Hytholt*

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(556) New approaches for gene and protein regulation

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, N-125B

Aditya Kunjapur, Chair
Xue Gao, Co-Chair

Sponsored by: Bioengineering

3:30 Paper 556a: Exploring *Streptococci* Cas9 Orthologs with Distinct PAM-Binding Motifs to Develop a Titratable Bacterial Gene Regulator — ***Yuxi Teng**, Jian Wang, Xinyu Gong, Jianli Zhang, Yifei Wu, Lei Lou, Michelle Li, zhong-Ru Xie, Yajun Yan*

3:48 Paper 556b: Programmable Synthetic Biomolecular Condensates for Cellular Control — ***Yifan Dai**, Ashutosh Chilkoti, Lingchong You*

4:06 Paper 556c: Engineered Prokaryotic Promoters Enable Multi-Input Processing Crispra/I Circuitry — ***Diego Alba**, Ryan Cardiff, Benjamin Tickman, Cholpisit Kiattisewee, Jesse Zalatan, James Carothers*

4:24 Paper 556d: Programmable Control of Protein Activity Via Reversible Formation of Biomolecular Condensates in Bacteria — *Mrugesh Parasa, Benjamin Rubino, Benjamin Howard, **Kevin Solomon***

4:42 Paper 556e: Optogenetically-Controlled Bacterial Persistence — ***Yousr Dhaouadi**, Dacheng Ren*

5:00 Paper 556f: Mapping the Sequence-Function Landscape for Quorum Sensing Specificity: Mitigating Signal Crosstalk of the Lasr Quorum Sensor for Programmable Bacterial Consortia — ***Min Zeng**, Vanessa Vu, Stephanie Call, Biprodev Sarker, Lauren B. Andrews*

5:18 Paper 556g: Approaching Sequence Completeness: Model-Predictive Design & Engineering of Synthetic Genetic Systems — ***Howard Salis***

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(557) KIChE-US Chapter Open Forum (Invited Talks)

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, N-228B

Seokjhin Kim, Chair
Su Ha, Co-Chair
Yoonjee Park, Co-Chair
Tae-Sik Oh, Co-Chair

Sponsored by: International Committee

3:30 Paper 557a: Amyloid Assembly: Unveiling Complexity and Tapping Engineering Opportunities — ***Jin Ryoun Kim***

3:55 Paper 557b: Next-Generation Sulfur Cathode: Electrocatalyst to Accelerate Sulfur Conversion Reaction — ***Jinwoo Lee***

4:20 Paper 557c: Polyolefins: From Reactors to Catalyst Sites — ***Kyu Yong Choi***

4:45 Paper 557d: Synthetic Protein Quality Control to Enhance Full-Length Translation in Bacteria — ***SangWoo Seo***

5:10 Paper 557e: Engineering Polymer Physics and Processing for Advanced Materials — ***Jay Park***

5:35 Paper 557f: Nanoconfinement-Induced Transitions from Linear to Non-Linear Dynamics of Condensed Matter Ranging from Biological to Geological Ones — ***Younjin Min***

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(558) Biomaterials for Drug Delivery I: Particle Platforms

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, N-121B

Jennifer Weiser, Chair
Lisa Volpatti, Co-Chair
Yichun Wang, Co-Chair
Rong Tong, Co-Chair

Sponsored by: Biomaterials

3:30 Paper 558a: miRNA Loading and Release Behavior of Dual Stimuli-Responsive Polycationic Nanoparticles in the Treatment of Glioblastoma Multiforme — ***Deidra Ward**, Nicholas Peppas*

3:47 Paper 558b: Varying Formulation Methods to Achieve Desired Diameter of Poly(caprolactone) Nanoparticles and Microparticles to Treat Disease — ***Claire Rowlands**, Ashbey Manning, Brittany Givens Rassoolkhani*

4:04 Paper 558c: Modulating Pegylation of Cationic Poly(amido amine) Dendrimers to Control Electrostatic-Based Drug Delivery to Articular Cartilage — ***Brandon Johnston**, Simone Douglas-Green, Joon Ho Park, Alan Grodzinsky, Paula T. Hammond*

4:21 Paper 558d: Functionalizing DNA Nanostructures for Vaccine and Therapeutic Materials Design — ***Grant Knappe**, Eike-Christian Wamhoff, Benjamin Read, Darrell J. Irvine, Mark Bathe*

4:38 Paper 558e: Engineering the Molecular Architectures of Antimicrobial Peptide (AMP)-Polymer Conjugates — ***Zixian Cui**, Kenneth Hawkins, Matthew Crawford, Debra Fisher, Molly Hughes, Rachel Letteri*

4:55 Paper 558f: Esterified Peptide Prodrugs for Nanocarrier Hitchhiking — ***Mark Bannon**, Spencer R. Marsh, Jane Jourdan, Robert G. Gourdie, Rachel Letteri*

5:12 Paper 558g: Genetically Engineered Cellular Nanoparticles for Targeted Drug Delivery — ***Liangfang Zhang***

5:47 Paper 558h: Scalable Fabrication of Endosomolytic Polymersomes for Cytosolic Delivery of Immunostimulatory Oligonucleotides — ***Payton Stone**, Hayden Pagendarm, Mina Aziz, Jessalyn Baljon, John Wilson*

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(559) Materials and Devices: From Energy Generation to Efficient Usage (Co-sponsored with Material Interfaces as Energy Solutions)

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, N-122A

Yuzhang Li, Chair
Matthew Panthani, Co-Chair
Andrej Lenert, Co-Chair
Carissa Eisler, Co-Chair

Sponsored by: Electronics and Photonics

3:30 Paper 559a: Controlling Phase Polydispersity and Crystal Orientation of Ruddlesden-Popper Perovskites for Efficient and Stable Solar Cells — ***Qiuming Yu***

4:00 Paper 559b: Low-Cost Composite Metallization to Reduce Cell-Crack-Induced Module Degradation — *Andre Chavez, April Jeffries, **Sang Han**, Sandra Huneycutt, Abasifreke Ebong, Duncan Harwood, Nicholas Azpiroz*

4:15 Paper 559c: Overcoming Loss Pathways in Photovoltaic Conversion of Thermal Radiation — ***Bosun Roy-Layinde***

4:30 Paper 559d: Fabrication of High-Performance Solution-Processed $AgInSe_2$ Semiconductor Thin-Films — ***Shubhanshu Agarwal**, David Rokke, Kyle Weideman, Rakesh Agrawal*

4:45 Paper 559e: Low Temperature Solution Processed Synthesis of Chalcogenide Perovskites Using Organometallic Precursors — ***Apurva Pradhan**, Jonathan Turnley, Shubhanshu Agarwal, Madeleine Uible, Shriya Khandelwal, Suzanne Bart, Rakesh Agrawal*

5:00 Paper 559f: A Facile, Catchall Pathway for Carbon Impurity Minimization Via Ligand Engineering of Colloidal $Cu(In_xGa_{1-x})S_2$ Nanoparticles for Thin-Film Photovoltaics — ***Daniel Hayes***, *Samantha Langdon, Rakesh Agrawal*

5:15 Paper 559g: Data Science Guided Experiments Identify Conjugated Polymer Solution Concentration As a Key Parameter in Organic Field Effect Transistor Device Performance — ***Rahul Venkatesh***, *Yulong Zheng, Campbell Viersen, Aaron Liu, Carlos Silva, Martha Grover, Elsa Reichmanis*

5:30 Paper 559h: Understanding the Structural Stability of Perovskites for Solar Energy Harvesting Using Molecular Dynamics Simulations in Comparison to Experiments — ***Barbara Morales***, ***Hendrik Heinz***

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(560) Polymer Networks and Gels II

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, N-122B

Kenneth Mineart, Chair
Jinhye Bae, Co-Chair
Xiaoguang Wang, Co-Chair

Sponsored by: Polymers

3:30 Paper 560a: Light-Induced Mechanical Response in Poly(alkylurea urethane) Networks Containing Azobenzene Compounds — ***William Lenart***, *Stuart J. Rowan*

3:45 Paper 560b: Characterizing the Formation of Strain-Induced Supramolecular Structures in Dynamic Polymer Networks — ***Christopher B. Cooper***, *Zhenan Bao*

4:00 Paper 560c: Macro to Micro: Emulating Natural Toughening Mechanisms in Multimorphic Soft Materials Via Orthogonal Interpenetrating Polymer Networks — ***Marshall Allen***, *Benny D. Freeman, Zachariah Page*

4:15 Paper 560d: Relationship between the Macroscopic Rheology and Shear-Induced Dynamics of Vitrimers — ***Fardin Khabaz***

4:30 Paper 560e: Loops, Links, and Bridges: Mechanical Properties of Triblock Copolymer Systems — ***Joshua Mysona***, *Juan De Pablo*

4:45 Paper 560f: The Influence of Tie-Molecules and Microstructure on the Fluid Solubility in Semi-Crystalline Polymers — ***Michele Valsecchi***, *Jona Ramadani, Amparo Galindo, George Jackson, Daryl Williams*

5:00 Paper 560g: Associations in Reversibly Bonded Networks — ***Scott Danielsen, PhD***, *Michael Rubinstein*

5:15 Paper 560h: Tunable, Phase-Separated Dynamic Networks through Thia-Michael Chemistry — ***Neil Dolinski***, *Ran Tao, Nicholas Boynton, Anthony Kotula, Charlie Lindberg, Aaron Forster, Stuart J. Rowan*

5:30 Paper 560i: Defining the Reactivity-Degradability Tradeoff for Cleavable Comonomers to Enable Degradation and Recycling of Thermoset Polymer Networks — ***David Lundberg***, *Jeremiah Johnson*

5:45: Break

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(561) Polymer Simulations: Methods and Applications

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, N-121C

Poornima Padmanabhan, Chair
Thomas Gartner III, Co-Chair
Wenlin Zhang, Co-Chair
Janani Sampath, Co-Chair
Dylan Anstine, Co-Chair

Sponsored by: Polymers

3:30 Paper 561a: Predicting Mixing Free Energy for Polymers with Atomistic Simulations — ***Puja Agarwala***, *Enrique D. Gomez, Scott T. Milner*

3:45 Paper 561b: Thermodynamic Modeling of the Polydispersity Influence on the Solubility of Ternary Semicrystalline Polymer-Solvent Systems — *Zengxuan Fan, Tim Zeiner,* ***Michael Fischlschweiger***

4:00 Paper 561c: An Efficient Hybrid Algorithm Combining Kinetic Monte Carlo and Continuum Model for Radical Polymerization — ***Yue Fang***, *Hanyu Gao*

4:15 Paper 561d: Coarse-Grain Models with a Parameterizable Friction Coefficient: Recovering Structure, Dynamics, and Viscosity in Polymer Melts — ***Lilian Johnson***, *Frederick Phelan Jr.*

4:30 Paper 561e: Coarse-Grained Modeling of Ion Transport in Salt-Doped and Single-Ion Block Copolymers — ***Lisa Hall***

5:00 Paper 561f: A Multiscale Strategy for Predicting Radiation Damage in Polymers — ***Matthew Kroonblawd***, *Anthony Yoshimura, Nir Goldman, Amitesh Maiti, James Lewicki, Andrew Saab*

5:15 Paper 561g: Investigating Effectiveness of Diethylhydroxylamine (DEHA) As Inhibitor for Oxygen-Involved Polymer Fouling Using Automatically Generated Multi-Phase Kinetics Model — ***Hao-Wei Pang***, *Michael Forsuelo, Xiaorui Dong, Ryan Hawtof, William Green*

5:30 Paper 561h: Multiscale Modeling of the Structure and Permeability of Self-Assembled Stratum Corneum Lipid Membranes — ***Christopher Iacovella***, *Parashara Shamaprasad, Chloe Frame, Annette Bunge, Clare McCabe*

5:45 Paper 561i: Refinement of Coarse-Grained Bonded Potential Dynamics in Chemically-Specific Molecular Dynamics Models of Polymers — *Lilian Johnson,* ***Frederick Phelan Jr.***

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(562) Two-Dimensional Materials and Thin Films

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, N-127B

Dongxia Liu, Chair
Seokjhin Kim, Co-Chair
Kumar Varoon Agrawal, Co-Chair

Sponsored by: Inorganic Materials

3:30 Paper 562a: Irreversible Synthesis of an Ultrastrong Two-Dimensional Polymeric Material — *Yuwen Zeng, Pavlo Gordiichuk, Takeo Ichihara, Ge Zhang, Emil Sandoz-Rosado, Eric D. Wetzel, Jason Tresback, Jing Yang, Daichi Kozawa, Zhongyue Yang, Matthias Kuehne,* ***Michelle Quien***, *Zhe Yuan, Xun Gong, Guangwei He, Daniel James Lundberg, Pingwei Liu, Albert Tianxiang Liu, Jing Fan Yang, Heather Kulik, Michael Strano*

3:45 Paper 562b: Solvent-Free Bottom-up Patterning of Zeolitic Imidazolate Frameworks — ***Dennis Lee***, *Yurun Miao, Matheus Dorneles de Mello, Mueed Ahmad, Mohammed Abdel-Rahman, Patrick Eckhert, Jorge Boscoboinik, Howard A. Fairbrother, Michael Tsapatsis*

4:00 Paper 562c: Investigating the Cof (Covalent Organic frameworks)-Graphene Interface Via Raman Spectroscopy and Optoelectronics — ***Roshan Nemade***, *Sungjoon Kim, Vikas Berry*

4:15 Paper 562d: Atomically Thin N-Based Graphene Membrane with Enhanced Adsorption and Size-Sieving Effect — ***Kuang Jung Hsu***, *Kumar Varoon Agrawal*

4:30 Paper 562e: Wetting Transparency of Single-Layer Graphene on Liquid Substrate — ***Fan Yang***, *Lei Li*

4:45 Paper 562f: Antiviral Mxene-Laser-Induced Graphene Composite Air Filters — *Meng-Qiang Zhao,* ***Botamina Moussa***

5:00 Paper 562g: Controlled expansion of pores in graphene at the Å-scale by CO2 — ***Kumar Varoon Agrawal***

5:15 Paper 562h: Integration of 2D Materials with Soft Matter for Multifunctional Robotic Materials — ***Po-Yen Chen***

5:30 Paper 562i: 2D Metal Carbides (MXenes) for Catalysis Applications — ***Yue Wu***

5:45 Paper 562k: 2D Zeolite Supported Metal Catalyst for Propane Ethane Dehydrogenation — ***Dongxia Liu***, *Antara Bhowmick*

(563) Nanotechnology approaches to diagnostics, implants, templating and assembly

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, W-104A

Margaret Bennewitz, Co-Chair
Rick Liao, Co-Chair

Sponsored by: Bionanotechnology

3:30 Paper 563a: Probing Brain Structure-Function Relationships in Neurodegeneration Using Organotypic Whole-Hemisphere Slice Models and Multiple Particle Tracking Technology — ***Brendan Butler***, *Elizabeth Nance*

3:55 Paper 563b: Long-Term Dose-Controllable Drug Delivery Implant — ***Yoonjee Park***, *Xingyu He, Zheng Yuan*

4:20 Paper 563c: Reconfiguration, Manipulation, and Control of Higher Order Dynamic DNA Origami Assemblies — ***Anjelica Kucinic***, *Teng Teng, Dylan Roderick, Ratnasingham Sooryakumar, Carlos E. Castro*

4:45 Paper 563d: Kinetic and Parametric Studies of Pd Mineralization on Barley Stripe Mosaic Virus (BSMV) Virus-like-Particles (VLPs) As Biotemplates — ***Chamath Vindula Basnayake Pussepitiyalage***, *Shohreh Hemmati, Akash J. Vaidya, Che-Yu Chou, Kevin Solomon, Michael T. Harris, Sue Loesch-Fries*

5:10 Paper 563e: Breast Cancer Specificity Assessment of Tumor Targeted Nano-, Encapsulated Manganese Oxide (NEMO) Particles — ***Celia Martinez de la Torre***, *Dhruvi Panchal, Kasey Freshwater, Margaret Bennewitz*

5:35 Paper 563f: Award Submission: Next-Generation Tattoo-Ink for Improved Endoscopic Imaging — ***Subhadeep Dutta***, *Jordan Yaron, Rahul Pannala, Kaushal Rege,* ***Mallikarjun Gosangi***

(564) Division Plenary: North American Mixing Forum Awards Session (Invited Talks)

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, N-229AB

Clara Gomez, Chair
Sujit Bhattacharya, Co-Chair
Justin Walker, Co-Chair

Sponsored by: North American Mixing Forum

3:30 Paper 564a: North American Mixing Forum Award Lecture: The Progression of Computational Fluid Dynamics As a Tool for Process and Equipment Design in Mixing — ***Eric E. Janz***

(565) Advances in Drug Discovery Processes (including HTE): Advanced Technology Approaches to Maximize Public Health Impacts

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, N-127A

Huiquan Wu, Chair
Curtis Martin, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

3:30 Paper 565a: CDER Efforts on Pharmaceutical Manufacturing Modernization — ***Stelios C. Tsinontides***

3:51 Paper 565b: Molecular Discovery with Limited Human Input Using a Machine Learning Guided Automated Platform — ***Matthew McDonald***, *Brent Koscher, Richard Canty, Seung Kyun Ha, Camille Bilodeau, Klavs Jensen*

4:12 Paper 565c: Computational Discovery of Peptide Inhibitors That Neutralize *C. Diff.* Toxin a in Jejunum and Colon Epithelial Cells — ***Sudeep Sarma***, *Xingqing Xiao, Stefano Menegatti, Nathan Crook, Scott Magness, Carol Hall*

4:33 Paper 565d: Identification of Resistance Determinants in Laboratory Evolved *Mycobacterium Smegmatis* evolved Under Temporally Variable Drug Profiles — ***Akanksha Kashyap***, *Sarika Mehra*

4:54 Paper 565e: Prediction of the Formation of Co-Amorphous Systems By Means of a Machine Learning Approach — ***Elisabeth Fink***, *Michael Brunsteiner, Amrit Paudel, Sarah Zellnitz-Neugebauer*

5:15 Paper 565f: Engineered Anti-CD276 Mab to Deliver Payload for Cancer Treatment — ***Yingnan Si***, *Xiaoguang Liu*

5:36 Paper 565g: A New Strategy for Persister Control — ***Sweta Roy***, *Zeynep Cakmak, Dacheng Ren*

(566) Advances in New Modalities: Biologics and Large Molecules

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, N-123

Moiz Diwan, Chair
Steve Rhieu, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

3:30 Paper 566a: Manufacturing of Aglycosylated Monoclonal Antibodies in Yeast — ***Neil C. Dalvie***, *Joseph R. Brady, Christopher Naranjo, Sergio Rodriguez Aponte, Ryan Johnston, J. Christopher Love*

3:51 Paper 566h: Online/At-line Optical Density-based Analytical Method to Quantify Empty-Full Adeno-associated Virus Particles — ***Srivatsan Ramesh***, *Ashton Lavoie, Amod Joshi, Jacob Irwin, Eric J. Yearley, Michael Guerrero*

4:12 Paper 566e: Tuning the Biophysical Properties of an IgG1-Based Antibody-Drug Conjugate By Traversing the Formulation Design Space — ***Sasha B. Ebrahimi***, *Xuan Hong, James Ludlow, Dany Doucet, Renuka Thirumangalathu*

4:33 Paper 566f: Mechanistic Insights into the Stabilization of Proteins By Saccharides — ***Johanna Dieplinger***, *Christina Moser, Joana Pinto, Amrit Paudel*

4:54 Paper 566g: A New Approach Towards the Production of a Personalizable Dry Solid Dosage Form for Biologics: In-Vial Direct Dosing and Drying By Inkjet Printing — ***Daniela Fiedler***, *Carolina Alva, Joana T. Pinto, Martin Spörk, Ramona Jeitler, Eva Roblegg*

(567) Pharma 4.0 (Advanced Controls, Process Automation, Data Analytics, etc.) in Drug Substance and Drug Product II

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, N-122C

Dominique Hebrault, Chair
Dana Barrasso, Co-Chair
Hossein Salami, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

3:30 Paper 567a: Pharma 4.0: Advanced Continuous Pharmaceutical Tablet Manufacturing Process — ***Ravendra Singh***

3:51 Paper 567b: Development of a DEM Based Digital Twin of a Tablet Press Feed Frame for the Evaluation of Continuous Manufacturing Control Strategies. — ***Johan Remmelgas***, *Dalibor Jajcevic, Peter Toson, Marko Matic, Michela Beretta, Jakob Rehrl, Julia Kruisz, Thomas O'Connor, Abdollah Koolivand, Geng Tian, Scott M. Krull, Johannes G. Khinast*

4:12 Paper 567c: Integrated System Modeling That Connects the Drug Product Manufacturing Process to Dissolution Testing — ***Indu Muthancheri***, *Marilyn Calderone, Nicolas Sanchez, Cecile Gabaude-Renou, Robert Yule*

4:33 Paper 567d: Hybrid Machine Learning Assisted Model Predictive Control of a Continuous Dry Granulation Tableting Line — ***Yan-Shu Huang***, *Rexonni Lagare, Sunidhi Bachawala, Marcial Gonzalez, Zoltan Nagy, Gintaras Reklaitis*

4:54 Paper 567e: Smart Process Analytics for the Prediction of Critical Quality Attributes in End-to-End Batch Manufacturing of Monoclonal Antibodies — ***Moo Sun Hong***, *Fabian Mohr, Chris Castro, Tom Mistretta, Roger A. Hart, Ben Smith, Richard D. Braatz*

5:15 Paper 567f: Characterizing the Freezing Process of Biopharmaceuticals in Vials at Commercial Scale: COVID-19 Vaccine Case Study and Mechanistic Modeling — ***Leif-Thore Deck***, *David R. Ochsenbein, Marco Mazzotti*

5:36 Paper 567g: Smart Data Analytics for Fault Detection and Its Application to Biopharmaceutical Manufacturing — ***Fabian Mohr***, *Weike Sun, Richard D. Braatz*

(568) Adsorption Processes for Energy Storage and Utilization

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, N-131A

James A. Ritter, Chair
Dipendu Saha, Co-Chair

Sponsored by: Adsorption and Ion Exchange

3:30 Paper 568a: Simultaneous Impregnation and Encapsulation of Silica Gel with Salt Hydrates for Thermal Energy Storage Applications — ***Suboohi Shervani***, *Curtis Strong, F Handan Tezel*

3:55 Paper 568b: Non-Vapor Compression Adsorptive Heating and Cooling Technology — ***James A. Ritter***, *K. James Hay, Armin Ebner*

4:20 Paper 568c: Use of Oat Hulls for Adsorption Based Thermal Energy Storage Applications — ***Suboohi Shervani***, *F Handan Tezel*

4:45: Break

5:10 Paper 568e: Bioenergy Production with Carbon Capture: An Optimization of Materials — ***Jackson Faylor***, *Edgar Ramirez Contreras, Kathy Tong, David Wagner*

(569) Advances in Fluid Particle Separations

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, N-131B

Jenifer Gomez Pastora, Chair
Oluwaseyi Odueyungbo, Co-Chair
Isaac Gamwo, Co-Chair

Sponsored by: Fluid-Particle Separations

3:30 Paper 569a: Hydrocyclone Separators: 1891-2022 and Beyond — ***Andre Benard***

3:50 Paper 569b: Magnetically-Enabled Recovery of Beads in Microchannels: Quadrupole Magnet Flow Sorters As Enhanced System Design — ***Cristina González-Fernández***, *Jenifer Gomez Pastora, Eugenio Bringas, Jeffrey Chalmers, Inmaculada Ortiz*

4:10 Paper 569c: Revealing Particle Transport Mechanisms in Microfiltration Processes Using Single-Particle Tracking — ***Haichao Wu***

4:30 Paper 569d: Magnetic Self-Assembly of Superparamagnetic Iron Oxide Nanoparticles Studied By in-Situ Small Angle X-Ray Scattering — ***Xian Wu***, *Jenifer Gomez Pastora, Jacob Strayer, Jeffrey Chalmers*

(570) Honorary Session for Prof. Ranil Wickramasinghe II

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, N-130

Raja Ghosh, Chair
Cristiana Boi, Co-Chair

Sponsored by: Bio Separations

3:30 Paper 570a: Opening Remarks for Honorary Session for Prof. Ranil Wickramasinghe II — ***Raja Ghosh***

3:51 Paper 570b: New Amine-Containing Facilitated Transport Membrane and Process for CO_2 Capture from Flue Gas — *Yang Han, Kai Chen, Witopo Salim, Dongzhu Wu,* ***W.S. Winston Ho***

4:12 Paper 570g: Modifying Synthetic Membranes: A Personal View — ***Georges Belfort***

4:33 Paper 570d: High Purification of Binary Protein Mixtures Having Close Molecular Weights By Ultrafiltration — ***Lixin Feng***, *Yufeng Song, Sagnik Basuray, Kamalesh Sirkar, Solomon Isu, Ranil Wickramasinghe*

4:54 Paper 570e: Applying the Method of Moments to Design Gradient Elution Chromatography — ***Andreas Seidel-Morgenstern***, *Hossam Abdelghani, Xinghai An, Shamsul Qamar*

5:15 Paper 570f: Remotely Controlled Magneto-Responsive Polymeric Membranes for Controlled Release of Biomacromolecules — ***Mathias Ulbricht***, *Mohamed Elleithy*

(571) Membranes for CO_2 Capture II

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, N-132A

Junyi Liu, Chair
Yang Han, Co-Chair
Nitesh Bhuwania, Co-Chair

Sponsored by: Membrane-Based Separations

3:30 Paper 571a: Nano-Confined Ionic Liquid Membrane for Highly Efficient CO_2 Capture from Flue Gas — ***Fan WANG***, *Huazheng LI, Huanghe Li, Weiwei Xu, Qiaobei Dong, Shiguang Li, Miao Yu*

3:51 Paper 571b: Elucidating the Role of Water in Amine-Facilitated CO_2 Transport Via Operando Transmission FTIR Spectroscopy — ***Sarah Pate***, *Hui Xu, Casey O'Brien*

4:12 Paper 571c: Polymer-Graphene Oxide Self-Assembled Membranes for H_2 Purification with Enhanced Selectivity for Carbon Capture Applications — *Giacomo Foli, Vincenzo Palermo,* ***Matteo Minelli***

4:33 Paper 571d: Tuning Ether Motifs in Polymers Membranes for Carbon Capture — ***Yasemin Basdogan***, *Zhen-Gang Wang*

4:54 Paper 571e: In-Silico Discovery of H_2/CO_2 Separation Potential of Mxene Membranes — *Sirin Massoumilari, Melih Doganci,* ***Sadiye Velioglu***

5:15 Paper 571f: A Green Solvent Incorporated Membrane Contactor Based Process for Energy-Efficient CO_2 Capture and Separation — ***Syed Islam***, *Md Arifuzzaman, Jingsong Huang, Jacek Jakowski, Rajeev Kumar, Gernot Rother, Vera Bocharova, Ramesh Bhave, Priyesh Wagh, David Sholl, Anisur Rahman, Tomonori Saito, Nirupam Aich, Alexei Sokolov*

5:36 Paper 571g: Process Design and Integration of Membrane-Cryogenic Distillation Based Hybrid Capture Systems for Hydrogen Production Process — ***Yongjae Song***, *Mun-Gi Jang, Jin-Kuk KIM*

(572) Molecular and Data Science Modeling of Adsorption I

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, N-131C

Gennady Gor, Chair
Daniel Siderius, Co-Chair
Yamil Colón, Co-Chair

Sponsored by: Adsorption and Ion Exchange

3:30 Paper 572a: Active Learning for Efficient Navigation of Adsorption Landscapes in MOFs — ***Krishnendu Mukherjee***, *Alexander Dowling, Yamil Colón*

3:45 Paper 572b: Adsorption Isotherms of Argon, Nitrogen, Carbon Dioxide, *n*-Butane, and Water for Pore Characterization of Chromatographic Particles — ***Chun-Kai Chang***, *Hsiao-Feng Liu, Joern Siepmann, Carlos Collados Cuadrado, Carola Schlumberger, Matthias Thommes, Mark R. Schure, Stephanie A. Schuster*

4:00 Paper 572c: Mofdb: An Accessible Online Database of Computational Adsorption Data for Nanoporous Materials — ***Scott Bobbitt***, *Kaihang Shi, Benjamin Bucior, Haoyuan Chen, Nathaniel Tracy-Amoroso, Zhao Li, Yangzesheng Sun, Julia Merlin, Joern Siepmann, Daniel Siderius, Randall Snurr*

4:15 Paper 572d: A Combined Deep Learning and Classical Potential Approach for Modeling Diffusion in Uio-66 — ***Siddarth Achar***, *Jacob Wardzala, Leonardo Bernasconi, Linfeng Zhang, Karl Johnson*

4:30 Paper 572e: Machine Learned Disposable Force Fields for Fluid-Solid Simulations: Application to Water Transport in Carbon and Boron-Nitride Nanotubes — ***Fabian L. Thiemann***, *Cristoph Schran, Patrick Rowe, Ondrej Marsalek, Angelos Michaelides, Erich A. Muller*

4:45 Paper 645e: Molecular Simulation of Compressibility of Water in Carbon Nanopores — ***Gennady Gor***, *Jason Ogbebor, Alexei Khalizov*

5:00 Paper 572g: Understanding and Virtual Design of Low-Volatility Ionic Liquid Solvents for Spacecraft CO_2 Separations — ***ISAAC Armstrong***, *Hendrik Heinz*

5:15 Paper 572h: Machine Learning Approach for Construction of Fingerprint Kernels for Pore Structure Characterization of Metal-Organic Frameworks — ***Shivam Parashar***, *Skandan Venkatraman, Alexander Neimark*

5:30 Paper 572i: High-Throughput Screening of Hypothetical Functionalized-Irmofs for Separation of Alkanes — ***Fangxi Wang***, *Abhishek Sose, Samrendra Singh, Sanket Deshmukh*

5:45 Paper 572j: Efficiently Exploring the Adsorption Space of Molecules in MOFs Combining the Use of Molecular Simulations, Machine Learning, and IAST — ***Xiaohan Yu***, *Sihoon Choi, Andrew Medford, David Sholl*

(573) Engineering Cancer II: Therapy

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, N-126C

Young Jik Kwon, Chair
Deisy Cristina Carvalho Fernandes, Co-Chair

Sponsored by: Chemical Engineers in Medicine

3:30 Paper 573a: Low Doses of Paclitaxel Induce a Dormant State in Brain Metastatic Breast Cancer Spheroids — ***Raghu Vamsi Kondapaneni***, *Rachel Warren, Shreyas Rao*

3:49 Paper 573b: Engineer CAR-Neutrophils for Targeted Cancer Immunotherapy — ***Xiaoping Bao***

4:08 Paper 573c: Immunogenic Treatment for Metastatic Breast Cancer Using Targeted Carbon Nanotube Mediated Photothermal Therapy in Combination with Anti-PD-1 — ***Gabriela Faria***, *Alexis Woodward, Clément G. Karch, Adam Aissanou, Roger Harrison*

4:27 Paper 573d: Immune Cell Homing Materials for Cancer Immunotherapy — ***Hua Wang***

4:46 Paper 573e: Electroporation and Cold Atmospheric Plasma As a Novel Cancer Treatment — ***Jordan Hoops***, *Kristen I. Haller, Mikaya M. Elliott, Rylie N. Andrews, Nicole Miller, Timothy Brenza, Prasoon K. Diwakar*

5:05 Paper 573f: Combined Gene and Chemotherapy for Cancer: Interdisciplinary Multimodal Approaches to Effective, Safe, and Diverse Therapies — ***Rebecca Lee***, *Cheng Wai "Winne" Lei, Margaret Lugin, Jee Young Chung, Woo Chang Hwang, Angela G. Fleischman, Namshik Han, Young Jik Kwon*

5:24 Paper 573g: The Landscape of Drug Sensitivity in Cancer Cell Lines Reveals Effective Drug Combinations for Cancer — ***Belinda Garana***, *Nicholas Graham*

5:43 Paper 573h: Multi-Modal Single-Cell Characterization As a Basis for Precision Therapy for Intratumoral Heterogeneity in Glioblastoma — ***James Park***, *Abdullah Feroze, Samuel Emerson, Anca Mihalas, C. Keene, Patrick Cimino, Adrian Lopez Garcia de Lomana, Wei-Ju Wu, Serdar Turkarslan, Kavya Kannan, Nitin Baliga, Anoop Patel*

(574) Low Dimensional Materials

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, N-227A

James Dorman, Chair
Letian Dou, Co-Chair

Sponsored by: Material Interfaces as Energy Solutions

3:30 Paper 574a: Exploring Protein-Nanocrystal Interfaces for Photoassisted Enzymatic Activity — ***Jennifer Cha***

4:05 Paper 574b: Determining Rate Constants for the Nucleation and Growth of Silver Nanowires Via the Polyol Method in a Batch and Millifluidic Reactor — ***Destiny Williams***, *Shohreh Hemmati, James Smay*

4:25: Break

4:45 Paper 574d: Synthesis and Stability of 2D Silicon Nanosheets — ***Matthew Panthani***

5:05 Paper 574e: Synthesis and Electronic Properties of Nanoparticles — ***Yuanbing Mao***

(575) Next-Gen Manufacturing in Pharma, Food, and Bioprocessing II

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, N-221A

Kristeen Esther Joseph, Chair
Manjiri Moharir, Co-Chair

Sponsored by: Next-Gen Manufacturing

3:30 Paper 575a: Multiscale Healthcare Supply Chains: Patient in the Loop — ***Miriam Sarkis***, *Niki Triantafyllou, Andrea Bernardi, Nilay Shah, Maria Papathanasiou*

3:51 Paper 575b: Knowledge-Informed Data-Driven Modeling for Robust Prediction of Microbial Inactivation in Food — ***Firnaaz Ahamed***, *Steve Zhang, Hyun-Seob Song*

4:12 Paper 575c: Systematic Design of Solvent Recovery Systems in Pharmaceutical Processes — *Jake Stengel,* ***Austin Lehr***, *Emmanuel Aboagye, John Chea, Kirti Yenkie, David Streather, Michael Parker, Claire MacLeod, Peter Schell*

4:33 Paper 575d: Quantifying the Intra-Sample Variability of Gelatinization of Starch Granules for Optimization of Food Processing — *Lanxin Mo, James Cheon,* ***John Frostad***

4:54 Paper 575e: Hybrid Modeling Using Universal Differential Equations for Lab-Scale Batch Production of β-Carotene Using *Saccharomyces Cerevisiae* — ***Mohammed Saad Faizan Bangi***, *Katy Kao, Joseph Kwon*

5:15 Paper 575f: Machine Learning-Based Modeling and Predictive Control of Crystallization Processes Under Batch-to-Batch Parametric Drift — ***Yingzhe Zheng***, *Tianyi Zhao, Xiaonan Wang, Zhe Wu*

5:36 Paper 575g: Models for Mammalian Cell Cultures Based on Long-Short Term Memory Recurrent Neural Networks — ***Satish Parulekar***, *Essa Almutar*

(576) Analysis and Assessment for Solving the Plastic Waste Crisis

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, N-121A

Robert Peters, Chair
Jeffrey Seay, Co-Chair

Sponsored by: Waste Plastics

3:30 Paper 576a: Leveraging Polymer Characterization to Gain Key Insights into Polyolefin Deconstruction Processes — ***Zachary Hinton***, *Thomas H. Epps III, LaShanda Korley*

3:51 Paper 576b: Microplastics in Foods and Beverages — ***Robert Peters***, *Larry Erickson*

4:12: Break

4:33 Paper 576d: Integrated Life Cycle and Techno-Economic Analysis Framework for Hydrothermal Liquefaction of Municipal Waste — ***Seshasayee Mahadevan Subramanya***, *Phillip E. Savage,* ***Rui Shi***

4:54 Paper 576e: Progress Towards to a Circular Plastic Economy: Intrinsic Kinetics of Polypropylene Pyrolysis Via Pulse-Heated Analysis of Solid Reactions (PHASR) — ***Nathan Sidhu***, *Isaac Mastalski, Paul Dauenhauer*

5:15 Paper 576f: Technoeconomic Analysis of Plastics Recycling Process Via Mechanocatalytic Reactions — ***Elisavet Anglou***, *Arvind Ganesan, William Bradley, Sankar Nair, Carsten Sievers, Fani Boukouvala*

5:36 Paper 576g: A Platform for Rapid Portable Analysis of Environmental Micro/Nano-Plastics — ***Eric Johnston***, *Victor Ugaz*

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(577) Advanced Electrochemical Energy Storage Technologies II

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, N-227B

Ling Fei, Co-Chair
Shuya Wei, Co-Chair

Sponsored by: Transport and Energy Processes

3:30 Paper 577a: Hydrogen Evolution Mitigation in Iron-Chromium Redox Flow Batteries Via Electrochemical Purification of the Electrolyte — ***Charles Wan***, *Kara Rodby, Mike Perry, Yet-Ming Chiang, Fikile R. Brushett*

3:50 Paper 577b: Theory of Layered-Oxide Cathode Degradation in Li-Ion Batteries By Oxidation-Induced Cation Disorder — ***Debbie Zhuang***, *Martin Z. Bazant*

4:10 Paper 577c: Low Cobalt NCM811 with Cobalt Gradient for Improved Structural Stability and Electrochemical Performance — ***Arjun Patel***, *Sourav Mallick, Mingyao Mou, Jethrine Mugumya, Michael L. Rasche, Herman Lopez, M. Parans Paranthaman, Mo Jiang, Ram Gupta*

4:30 Paper 577d: Batch and Slug-Flow Synthesis of NMC111 Precursor Micro Crystals for Battery Application: A Comparative Study — ***Jethrine Mugumya***, *Mingyao Mou, Arjun Patel, Sourav Mallick, Michael L. Rasche, Ram Gupta, Mo Jiang*

4:50: Break

5:00 Paper 577e: High Power Symmetric Zinc Iodine Redox Flow Batteries with Functionalized Carbon Electrodes — ***Abena Williams***, *Robert Emmett, William Marcengill, Mark E. Roberts*

5:20 Paper 577f: Electrochemical-Mechanical Microstructure-Scale Battery Modeling for Improved Performance and Degradation Predictions during Fast Charging. — ***Francois Usseglio Viretta***, *Hari Sitaraman, Michael Brazell, Jeffery Allen, Marc Day, Kandler Smith*

5:40 Paper 577g: A Molecular Simulation Study of the Solvation and Selectivity of Glycerol-Based Solvents for Different Cationic Species. — ***Gabriel Barbosa***, *Jason Bara, C. Heath Turner*

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(578) William R. Schowalter Lecture

Wednesday, Nov 16, 6:15 PM
Phoenix Convention Center, North Ballroom 120D

Pablo Debenedetti, Chair

Sponsored by: Awards Committee

6:15 Paper 578a: From Particles to People and Complex Organizations — ***John L. Anderson***

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(580) Biomass Conversion III: Biomass Processing & Sugar Chemistry

Thursday, Nov 17, 8:00 AM
Phoenix Convention Center, N-128A

Konstantinos Goulas, Chair
Brandon O'Neill, Co-Chair
Ana Colaco Morais, Co-Chair

Sponsored by: Catalysis

8:00 Paper 580a: Bio-Based Amphiphile Preparation through Aldehyde Assisted Lignocellulosic Biomass Fractionation — ***Songlan Sun***, *Gaia de Angelis, Stefania Bertella, Graham Dick, Esther Amstad, Jeremy Luterbacher*

8:18 Paper 580b: Multi-Pass Flow-through Reductive Catalytic Fractionation Enables Minimal Solvent Usage — ***Jun Hee Jang***, *David Brandner, Yuriy Roman, Gregg T. Beckham*

8:36 Paper 580c: Syngas Quality Improvement through ZSM-5 Supported Iron Oxide Oxygen Carrier in Chemical Looping Gasification of Biomass with Enhanced Conversion and CO_2 Capture — ***Afsaneh Khajeh***, *Hessamedin Naeimi, Lijun Wang, Abolghasem Shahbazi*

8:54 Paper 580d: Integrated Pathway for the Efficient Conversion of Lignocellulosic Sugars to HMF — ***Ravikumar Gogar***, *Sridhar Viamajala, Patricia Relue, Sasidhar Varanasi*

9:12 Paper 580e: Selective Glucose Isomerization to Fructose Using a Heterogeneous Immobilized Tertiary Amine with Tuned Molecular Design — ***Nicholas Brunelli***, *Ashwin Kane, Nitish Deshpande*

9:30 Paper 580f: Catalytic Fundamentals of Renewable Hydrogen Production from Aqueous Phase Reforming: Active Sites, Solvent Effects, and Deactivation — ***Bryan Hare***, *Ricardo Garcia Carcamo, Rachel Getman, Carsten Sievers*

9:48 Paper 580g: Simultaneous Vibrational Spectroscopic Monitoring of Glucose Transformation — ***Jakub Konkol***, *George Tsilomelekis*

10:06 Paper 580h: Deep Reaction Network of Glucose Pyrolysis: Discovering Unexpected Intermediates and Reaction Mechanisms — ***Qiyuan Zhao***, *Brett Savoie*

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(581) Catalysis on Low Dimensional Materials : 2D Catalysts

Thursday, Nov 17, 8:00 AM
Phoenix Convention Center, N-127A

Prashant Deshlahra, Chair
Tej Choksi, Co-Chair

Sponsored by: Catalysis

8:00 Paper 581a: Photo-Catalytic Treatment of Perfluoroalkyl Substances (PFAS) over Hexagonal Boron Nitride — *Yu Chen,* ***Thomas Senftle***

8:20 Paper 581b: Probing the Catalytic Activity of Nitride Mxenes in Real Time — *Denis Johnson, Kyle Hansen, Ray Yoo,* ***Abdoulaye Djire***

8:50 Paper 581c: Electrostatic Manipulation of Lewis Acidity in Ultrathin Catalytic Films Via Programmable Catalytic Condensers — ***Sallye R. Gathmann***, *C. Daniel Frisbie, Paul Dauenhauer*

9:10 Paper 581d: Universal Properties of Metal-Supported Oxide Films from Scaling Relationships: Elucidation of Strong Metal Support Interactions. — ***Kaustubh Sawant***, *Junxian Gao, Dmitry Zemlyanov, Zhenhua Zeng, Jeffrey T. Miller, Jeffrey Greeley*

9:30 Paper 581e: 2D Hierarchical Zeolites: Facile Synthesis and Catalysis Applications — ***Dongxia Liu***

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(582) Data Science & Machine Learning Approaches to Catalysis III: Applications of Machine Learning to Heterogeneous Catalysis: From Porous Materials to Cluster Catalysis

Thursday, Nov 17, 8:00 AM
Phoenix Convention Center, N-128B

Hongliang Xin, Chair
Konstantinos Alexopoulos, Co-Chair

Sponsored by: Catalysis

8:00 Paper 582a: Crystal Engineering of a Zeolite Using Machine Learning — ***Xinyu Li***, *He Han,* ***Nikolas Evangelou***, ***Noah J. Wichrowski***, *Peng Lu, Wenqian Xu, Son-Jong Hwang, Wenyang Zhao, Chunshan Song, Xinwen Guo, Aditya Bhan, Ioannis G. Kevrekidis, Michael Tsapatsis*

8:18: Break

8:36 Paper 582c: Electronic Environment-Based Correction Scheme Using DFT and Wft-Level Energies to Accurately Predict Energetics of Catalytic Interfaces — ***Sushree Jagriti Sahoo***, *Xiangyun Lei, Andrew Medford*

8:54 Paper 582d: Computational Design of Metal Oxide Nanoclusters for Selective Partial Oxidation of Hydrocarbons — ***Xijun Wang***, *Randall Snurr*

9:12 Paper 582e: Predicting Thermochemical Properties of Hydrocarbon Adsorbates on Metal Surfaces Using Machine Learning — ***Jinwoong Nam***, *Charanyadevi Ramasamy, Daniel Raser, Gustavo Barbosa Couto, Fuat Celik*

9:30 Paper 582f: A Data-Driven Approach Towards Assessing the Stability and Activity of Nanoparticles Containing on Order of Thousand Atoms: A Case Study Using the Oxygen Reduction Reaction — ***Kah Meng Yam***, *Asmee Prabhu, Mun Ling Lee, Wern Chin Chan, Tej Choksi*

9:48 Paper 582g: Modeling the Distribution of Supported Sub-Nanometer Cluster Catalysts — ***Salman A. Khan***, *Stavros Caratzoulas, Dionisios Vlachos*

10:06 Paper 582h: Site Geometry Driven Selective Hydrogenation on Intermetallic Catalysts — ***Unnatti Sharma***, *Angela Nguyen, Zachary Ulissi, Michael J. Janik*

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(583) Electrocatalysis III: Fundamental

Thursday, Nov 17, 8:00 AM
Phoenix Convention Center, N-127C

Ian McCrum, Chair
Brian Tackett, Co-Chair

Sponsored by: Catalysis

8:00 Paper 583a: The Good, the Bad and the Ugly of Combining Theory, Spectroscopy and Experimental Kinetic Studies in Fundamental Electrocatalysis. — ***Carlos Morales-Guio***

8:24: Break

8:42 Paper 583c: Structure-Activity-Stability Investigation of Transition Metal Antimonate Oxynitride and Oxysulfide Oxygen Reduction Nanoparticle Electrocatalysts — ***Gaurav A. Kamat***, *Melissa Kreider, Michaela Burke Stevens, Thomas Jaramillo*

9:00 Paper 583d: Tuning Single Atom Dopants on Manganese Oxide for Selective Electrocatalytic Olefin Epoxidation — ***Minju Chung***, *Kyoungsuk Jin, Karthish Manthiram*

9:18 Paper 583e: Toward a Fundamental Understanding of Catalytically-Active Phases and Reaction Mechanism of Layered Double Hydroxides for the Oxygen Evolution Reaction — ***Zhenhua Zeng***, *Fabio Dionigi, Peter Strasser, Jeffrey Greeley*

9:36 Paper 583f: Electrocatalytic Transformation of Organic Substrates — ***Christine Lucky***, *Taobo Wang, Marcel Schreier*

9:54 Paper 583g: Accelerating Electrocatalyst Discovery and Understanding with the Open-Access Grand-Canonical Beast Database — ***Nick Singstock***, *Charles B. Musgrave*

10:12 Paper 583h: Ethane Electrochemical Oxidative Dehydrogenation: Impact of Electrocatalyst Tuning and Feedstock Composition — ***Andrew Kasick***, *Ahmad Abu Hajer, Damilola Daramola, Jason Trembly*

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(584) Reaction Chemistry and Engineering I

Thursday, Nov 17, 8:00 AM
Phoenix Convention Center, N-127B

Milad Abolhasani, Chair
Manish Shetty, Co-Chair

Sponsored by: Reaction Engineering

8:00 Paper 584a: Prototyping Egg-Yolk and Egg-White Catalyst Pellets for Exothermic Reactions — ***Ronny Tobias Zimmermann***, *Jens Bremer, Kai Sundmacher*

8:18 Paper 584b: Elucidating the Acidity-Activity Relation in Sulfated Metal Oxides for the Solvent-Free Tert-Butylation of Phenol — ***Adam Zuber***, *George Tsilomelekis*

8:36: Break

8:54 Paper 584d: Use of Reaction Modeling and on-Line Liquid Chromatography at Pilot Plant Scale to Obtain Mechanistic Insights — ***Arnav Malkani***, *Zhihao Lin, Kaitlyn Brinza, Yong-Li Zhong, Paul Dunk, Victoria Zhang, Latevi Lawson, Daniel DiRocco, Jonathan McMullen*

9:12 Paper 584e: Analyzing the Performance of Uncoupled Mode Approximations in Reaction Rate Calculations — ***Shih-Cheng Li***, *Yen-Chun Lin, Yi-Pei Li*

9:30 Paper 584f: Recent Progress in the Creation of Virtual Plants for Gas-Liquid Processes in API Manufacture — ***Christopher Hone***, *C. Oliver Kappe*

9:48 Paper 584g: Identifying the Oxidation Kinetics from Fe Doped Magnesium Manganate Systems — ***Jayni Hashimoto***, *Alicia Bayon, Olivia Tamburro, Vivienne Pelletier, Christopher L. Muhich*

10:06 Paper 8b: Continuous Flow Calorimetry for the Thermal Characterization of Highly Exothermic and Fast Reactions — ***Christopher Hone***, *Gang Fu, Dominik Polterauer, C. Oliver Kappe*

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(585) Practical Applications of Computational Chemistry and Molecular Simulation for Polymers and Biological Systems

Thursday, Nov 17, 8:00 AM
Phoenix Convention Center, N-222B

Christopher Muhich, Chair
Steven G. Arturo, Co-Chair
Sukrit Mukhopadhyay, Co-Chair
Jonathan Moore, Co-Chair
Andrea R. Browning, Co-Chair
Martin Sanborn, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

8:00 Paper 585a: Structure Enumeration Algorithm for Silicone Mq-Resins — ***Steven G. Arturo***, *Thomas D. Bekemeier, Don Eldred, Wei Gao, James H. Wade, Tianlan Zhang*

8:30: Break

8:50 Paper 585c: Force Fields for the Prediction of Transport Properties of Lubricants at Extreme Conditions — ***Sebastian Schmitt***, *Simon Stephan, Hans Hasse*

9:10 Paper 585d: Understanding Electronic Properties of 1-n-Alkyl-3-Methylimidazolium Chloride Ionic Liquids with Iron Porphyrin — ***Sudip Kumar Das***, *Jindal Shah*

9:30 Paper 585e: Applying Deep Learning to Accelerate Molecular Dynamics Simulation-Based Structural Properties Prediction for Biomolecules. — ***Pin-Kuang Lai***

9:50 Paper 585f: Comparison of Dissociation Kinetics and Mechanism of Classical and Non-Classical Cannabinoids from Cannabinoid Receptors — ***Soumajit Dutta***, *Diwakar Shukla*

10:10 Paper 585g: Indacenodinaphthothiophene Isomers with Polyradical Character — ***Md Abdus Sabuj***, *Md Masrul Huda, Chinmoy Saha, Neeraj Rai*

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(586) Applied Math for Biological Systems: Plants and Microbes

Thursday, Nov 17, 8:00 AM
Phoenix Convention Center, W-101C

Mohammad Mazharul Islam, Chair
Kiumars Badr, Co-Chair

Sponsored by: Applied Mathematics and Numerical Analysis

8:00 Paper 586a: Trick and Treat: Pulse Dosing to Eradicate Persister Bacteria — ***Garima Singh***, *Mehmet Orman, Jacinta C. Conrad, Michael Nikolaou*

8:19 Paper 586b: Analysis of Stress-Induced H_2O_2 Signaling Waveforms *in Planta* — ***Thomas Porter***, *Michael N. Heinz, Daniel James Lundberg, Allan M. Brooks, Tedrick Thomas Salim Lew, Kevin Silmore, Volodymyr Koman, Mervin Ang, Duc-Thinh Khong, Gajendra Pratap Singh, James Swan, Rajani Sarojam, Nam-Hai Chua, Michael Strano*

8:38 Paper 586c: Discovery of Inhibitors for Mura Protein As Antimicrobials through an Integrated Computational and Experimental Approach — *Fangyuan Zhang, Joshua Graham, Tianhua Zhai, Yanhong Liu,* ***Zuyi Huang***

8:57 Paper 586d: Building Bottom-up Kinetic Models for Optimizing Cell-Free Lignocellulose Degradation Systems — ***Wheaton Schroeder***, *Daniel Olson, Costas D. Maranas*

9:16 Paper 586e: Structure-Guided Metabolic Modeling of Non-Model Organisms — ***Ratul Chowdhury***

9:35 Paper 586f: Comparative Structural Analyses of Antimicrobial Resistant *K. Pneumoniae* metabolic Networks Via Stochastic Block Modeling and Machine Learning — ***Victoria Jones***, *Prodromos Daoutidis*

9:54 Paper 586g: Understanding the Redox Shift in a *Clostridium Tyrobutyricum* mutant Strain for Butanol Production through Genome-Scale Metabolic Modeling — ***Kiumars Badr***, ***Loyal Murphy***, *Yi Wang, Jin Wang*

10:13 Paper 586h: Identifying Thermodynamic Bottlenecks Caused By Osmotic Stress in the Genome-Scale Metabolic Model of Escherichia coli — ***Alexandre Tremblay***, *Pavlos Stephanos Bekiaris, Philipp Schneider, Radhakrishnan Mahadevan, Steffen Klamt*

(587) Modeling, Control, and Optimization of Energy Systems I

Thursday, Nov 17, 8:00 AM
Phoenix Convention Center, W-101B

Matthew Ellis, Chair
Yuhe Tian, Co-Chair

Sponsored by: Systems and Process Control

8:00 Paper 587a: Nonlinear Model Predictive Control for Solid Oxide Electrolysis Cells — ***Vibhav Dabadghao***, *Douglas A. Allan, John C. Eslick, Debangsu Bhattacharyya, Lorenz Biegler*

8:19 Paper 587b: Economic Model Predictive Control of Integrated Energy Systems: A Multi-Time-Scale Framework — ***Long Wu***, *Xunyuan Yin, Lei Pan, Jinfeng Liu*

8:38 Paper 587c: A Data-Driven Model Predictive Control Framework for Optimal Charging of Li-Ion Batteries with Experimental Validation — ***Bhavana Bhadriraju***, *Jooyoung Lee, Choongho Yu, Joseph Kwon, Faisal Khan*

8:57 Paper 587d: Model Predictive Control for a Large-Scale Chemical Looping Combustion System in a Packed Bed Reactor — *Kathryn Toffolo, Sarah Meunier,* ***Luis Ricardez-Sandoval***

9:16 Paper 587e: Cloud-Based Economic Model Predictive Control for Residential Heat Pump Water Heaters — ***Loren dela Rosa***, *Caton Mande, Matthew Ellis*

9:35 Paper 587f: Model Predictive Control of Green-Powered Zero Waste Urban Plant Factories for Sustainable Food Production — *Patrick Hinkel,* ***Davood Babaei Pourkargar***

9:54 Paper 587g: Modeling and Optimization of Carbon-Negative Ngcc Plant Enabled By Modular Direct Air Capture — ***Pengfei Cheng***, *David Thierry, Matthew Realff, Joseph K. Scott*

10:13 Paper 587h: Feasibility Analysis of a Membrane System for Direct Air Capture of CO_2 — ***Vitor Gama***, *San Dinh, Oishi Sanyal, Fernando V. Lima*

(588) Process Monitoring & Fault Detection

Thursday, Nov 17, 8:00 AM
Phoenix Convention Center, W-101A

Ravendra Singh, Chair
Davood Babaei Pourkargar, Co-Chair

Sponsored by: Information Management and Intelligent Systems

8:00 Paper 588a: Optimal Hierarchical Stationarity Feature Extraction for Monitoring Start-up Intermittent Manufacturing — *Yan Qin,* ***Xunyuan Yin***

8:19 Paper 588b: Optimal Sensor Network Design and State Estimation of Nonlinear Differential Algebraic System: Application to Corrosion Monitoring in a Power Plant Boiler — ***Chandra Sekhar Somayajula***, *Debangsu Bhattacharyya, Xingbo Liu, Shanshan Hu*

8:38 Paper 588c: Discovery of Cyclic Loops in Bayesian Network for Root Cause Diagnosis of Process Faults — ***Pallavi Kumari***, *Qingsheng Wang, Faisal Khan, Joseph Kwon*

8:57 Paper 588d: Alarm and Safety System Design Using Forward Flux Sampling — ***Vikram Sudarshan***, *Warren Seider, Amish J. Patel, Ulku Oktem, Jeffrey E. Arbogast*

9:16 Paper 588e: Disturbance Decoupled Functional Observers for Simultaneous Fault Detection and Estimation in Nonlinear Systems — ***Costas Kravaris***, *Sunjeev Venkateswaran, Benjamin Wilhite*

9:35 Paper 588f: An Advanced Set-Based Fault Diagnosis Approach for Uncertain Nonlinear Chemical Systems — ***Bowen Mu***, *Joseph K. Scott*

9:54 Paper 588g: Online Steady and Transient State Detection Using the Dickey-Fuller Test — ***Evren Turan***, *Johannes Jäschke*

10:13 Paper 588h: Process Monitoring Optimization Via Unsupervised Clustering Metrics — ***Luis Briceno-Mena***, ***Zachary Webb***, *Jose A. Romagnoli*

(589) Interfacial Phenomena in Electrochemical and Electrokinetic Systems

Thursday, Nov 17, 8:00 AM
Phoenix Convention Center, N-232C

Ariel Furst, Chair
Patricia Taboada-Serrano, Co-Chair

Sponsored by: Interfacial Phenomena

8:00 Paper 589a: Probing the Electrical Double Layer in Highly-Concentrated Salt Environments — ***Sarah Berlinger***, *Zachary Lamberty, Joelle Frechette*

8:15 Paper 589b: Transport in Electrochemical Capacitors: Effects of Porous Geometry, Electrolyte Asymmetry, and Redox Reactions — *Filipe Henrique, Nathan Jarvey,* ***Ankur Gupta***

8:30 Paper 589c: Concentration Gradient Generation Using Spatially Non-Uniform AC Electric Fields — ***Ran An***, *Adrienne Minerick*

8:45 Paper 589d: Transient Kinetic Isotope Effects Reveal Interfacial CO_2 Dissolution Kinetics — ***Max Huelsey***, *Yogesh Surendranath*

9:00 Paper 589e: Illustrating the Significance of Π-Electrons in the Adsorption of Corrosion Inhibitors — ***Ahmed Mohamed***, *Donald Visco Jr., David M. Bastidas*

9:15: Break

9:30 Paper 589g: Investigating Metal Dissolution of Calcium Iridium Oxide during Long-Term Oxygen Evolution Reaction in Acid — ***Ruihan Li***, *Linsey Seitz*

9:45 Paper 589h: Ptoh Induced Strain on Pt(111) during Chronoamperometry between 0.6 and 1.1 V_{RHE}: Influence on the Pt(111) Interface and Catalytic Reactivity — ***Arthur Shih***, *Kasinath Ojha, Mingchuan Luo, Xiaoting Chen, Guangdong Liu, Zhiqin Liang, Matias Viallalba, Francesc Valls Mascaró, Hassan Javed, Rafaël Vos, Huiqiu Deng, Jeffrey Greeley, Zhenhua Zeng, Marc T.M. Koper*

(590) Special Topics in Colloids

Thursday, Nov 17, 8:00 AM
Phoenix Convention Center, N-232B

Marina Tsianou, Chair

Sponsored by: Interfacial Phenomena

8:00 Paper 590a: Gold Nanoparticle Colloidal Catalysts: Role of Ligands and Strategies for Recovery and Reuse — ***Christopher Kitchens***

8:15 Paper 590b: Nanoengineering of Cellulose Nanocrystals for Enhanced Aqueous Redispersibility — ***Mica Pitcher***, *Amir Sheikhi, Breanna Huntington*

8:30 Paper 590c: Hybrid Membranes Based on the Controlled Assembly of Gelatin-Stabilized Amorphous Calcium Phosphate and $Ti_3C_2T_x$ Mxene Nanoflakes — *Gelareh Rezvan, Mary Walden, Farivash Gholamirad, Monirosadat Sadati,* ***Nader Taheri-Qazvini***

8:45 Paper 590d: Fundamentals of Calcium Carbonate Scale Formation in Oil-Water Emulsions — ***Shang-Lin Yeh***, *Amir Sheikhi*

9:00 Paper 590e: Wettability Alteration of Carbonate Rock By Gemini Surfactants — *Xiao Deng,* ***Muhammad Shahzad Kamal***, *Syed Hussain, Shirish Patil, Mohamed Mahmoud, Emad W. Al Shalabi, Dhafer Al-Shehri, Anas Hassan*

9:15 Paper 590f: Effect of Brine and Organic Acids on Initial Wettability of Carbonate Rocks — ***Sikandar BIND***, *Himanshu Sharma*

9:30 Paper 590g: Effect of Brine & Oil Composition on Wettability of Carbonate Rocks — ***Sikandar BIND***, *Himanshu Sharma*

9:45 Paper 590h: On the Mechanism Metal Nanoparticle Synthesis in Dendrimers — ***Sanjeev Kumar***, *Hariharan A*

(591) Thermodynamics at the Nanoscale

Thursday, Nov 17, 8:00 AM
Phoenix Convention Center, N-222C

Erik Santiso, Chair

Sponsored by: Thermodynamics and Transport Properties

8:00 Paper 591a: Structure of Water in Supramolecules of Different Functionalization — ***Busayo Alagbe***, *Bruce C. Gibb, Henry Ashbaugh*

8:18 Paper 591b: Thermodynamic Evidence for Type II Porous Liquids — ***Isaiah Borne***, *Kartik Saigal, Christopher W. Jones, Ryan P. Lively*

8:36 Paper 591c: Crystallization of Soft Cuboidal Blue Phase Liquid Crystals in Shells — *Sepideh Norouzi, Antonio Tavera-Vazquez, Johanan Ramirez-de Arellano, Teresa Lopez-Leon, Jose A. Martinez-Gonzalez, Juan De Pablo,* ***Monirosadat Sadati***

8:54 Paper 591d: Elucidating the Effect of Ionic Liquid Structure on the Separation of Hydrofluorocarbon Mixtures: A Molecular Modeling Study — ***Ning Wang***, *Yong Zhang, Ryan S. DeFever, Edward Maginn*

9:12 Paper 591e: Frank Elastic Constants of Semi-Flexible Polymer Nematic Solutions — ***Ashesh Ghosh***, *Quinn MacPherson, Zhen-Gang Wang, Andrew Spakowitz*

9:30 Paper 591f: A Model to Describe Associating Mixtures of Structural Isomers — *Gottfried Segner, Patrick Zimmermann,* ***Tim Zeiner***

9:48 Paper 591g: Functionalized Nanoporous Graphene As a Candidate for Selective Water Evaporation from Ionic Solutions — ***Anshaj Ronghe***, *K. G. Ayappa*

10:06 Paper 591h: Phase Field Simulation for Rapid Solidification Couple with Solute Diffusion of Al-Cu Binary Alloy — ***Atiqur Rahman***, *Pabitra Choudhury*

(592) Design and Analysis of Carbon Capture and Negative Emissions Technologies - Experimental

Thursday, Nov 17, 8:00 AM
Phoenix Convention Center, N-225B

Dora Lopez De Alonzo, Chair
Omar J. Guerra, Co-Chair
Toufiq Reza, Co-Chair

Sponsored by: Climate Change

8:00 Paper 592a: Biomass Cofiring with Precombustion Carbon Capture Baseline Testing at Und Eerc — ***Joshua Stanislowski***

8:21 Paper 592b: Investigating Oxidative Degradation Products and Mechanisms of Aminopolymer Sorbents for Direct Air Capture (DAC) — ***Yoseph Guta***, *Juliana Carneiro, Giada Innocenti, Simon H. Pang, Miles Sakwa-Novak, Christopher W. Jones, Carsten Sievers*

8:42 Paper 592c: Quaternary Ammonium Functionalized Poly(arylene ether sulfone) Copolymers for Direct Air Capture — ***Hoda Shokrollahzadeh Behbahani***, *Matthew D. Green*

9:03 Paper 592d: Synthesizing DAC Hydrophobic Polymers with Various Form Factors — ***Ani Nazari***, *Matthew D. Green*

9:24 Paper 592e: Sorbent Regeneration Energy Analysis of Phase-Changing Guanidine-Based Ligands Used for CO_2 Direct-Air Capture — ***Abishek Kasturi***, *Sotira Yiacoumi, Diana Stamberga, Radu Custelcean, Costas Tsouris*

9:45 Paper 592f: Effect of Fundamental Biopolymers in the Development of Surface Porosity and CO_2 capture Capacity of Superactivated Hydrochars — ***Al Ibtida Sultana***, *Toufiq Reza*

10:06 Paper 592g: Performance Evaluation of Membrane Module for CO_2 Separation from Ambient Air — ***Palash Panja***, *Maksudul Alam, Milind Deo*

(593) Environmental Issues involving Biochar

Thursday, Nov 17, 8:00 AM
Phoenix Convention Center, N-225A

Jeffrey Seay, Chair
Alvaro Orjuela, Co-Chair

Sponsored by: Sustainability

8:00 Paper 593a: Adsorption of Microcystin-LR on Biochar Studied Using Molecular Simulations — ***Hemant Nagar***, *Toufiq Reza, Nirupam Aich, Sumit Sharma*

8:25 Paper 593b: Thermochemical Conversion in Space: Developing Mars Regolith- Activated Hydrochar Composite for Enhanced Water Retention in Mars — ***Al Ibtida Sultana***, *Toufiq Reza*

8:50 Paper 593c: Optimization of Pyrolysis Parameters for Biochar Production — ***Aviv Kresch***, *David Jiang, Xiao Lin, Amanda Simson*

9:15 Paper 593d: Effect of Surfactant on HTL Derived Hydrochar Physicochemical Characteristics — ***Khang Huynh***, *Bharathkiran Maddipudi, Anuradha Shende, Rajesh Shende*

(594) Advances in Metabolic Engineering- Prokaryotic Organisms

Thursday, Nov 17, 8:00 AM
Phoenix Convention Center, N-125A

Andrew Jones, Chair
Joshua Michener, Co-Chair

Sponsored by: Bioengineering

8:00 Paper 594a: Engineering Medium Chain Fatty Acid Production in *Synechococcus Sp.* PCC7002 — ***Joshua P. Abraham***, *Baltazar E. Zuniga, Miles N. Crockett, Hawkins Shepard, Jody C. May, John McLean, Jamey Young, Brian F. Pfleger*

8:18 Paper 594b: Bioproduction of Aromatic Amines Enabled By Stress-Resistant Bacteria — ***Cholpisit Kiattisewee***, *Ian Faulkner, Jesse Zalatan, James Carothers*

8:36 Paper 594c: Genomic Engineering of *Escherichia coli* for Improved Aromatic Aldehyde Stability — ***Neil Butler***, *Shelby Anderson, Roman Dickey, Michaela Jones, Ishika Govil, Aditya Kunjapur*

8:54 Paper 594d: Screening of Norbaeocystin Methyltransferase Variants Enables Enhanced Psilocybin and Baeocystin Production in *E. coli* — ***Madeline McKinney***, *J. Andrew Jones*

9:12 Paper 594e: Natural Product Synthesis from Lignin Aromatics Using *Acinetobacter Baylyi* ADP1 — ***Bradley Biggs***, *Keith Tyo*

9:30 Paper 594f: The Metabolic Engineering of *E. coli* for N-Glycolyl Chondroitin Production — ***Adeola Awofiranye***, *Ke Xia, Sultan N. Baytas, Robert J. Linhardt, Mattheos Koffas*

9:48 Paper 594g: Inducible Directed Evolution of Multigene Pathways in E. coli — ***Nathan Crook***

(595) Micro- and Nano-Scale Technologies in Life Sciences II

Thursday, Nov 17, 8:00 AM
Phoenix Convention Center, N-126A

Christina Bailey-Hytholt, Chair
Bomyi Lim, Co-Chair
Whitney Stoppel, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

8:00 Paper 595a: Effectiveness of Engineered Nanoceria at Inhibiting Thermally-Induced Oxidative Stress in Symbiodinium. — *Liza M. Roger, Joseph A. Russo, Robert Jinkerson, Juan Pablo Giraldo,* ***Nastassja Lewinski***

8:18 Paper 595b: Soft Poly-Ethylene-Glycol (PEG) Micelles and Lipid Nanoparticles (LNPs) Resolve Autophagy and Reduce Pro-Inflammatory Cytokine Secretion in RAW264.7 Murine Macrophages — *Monireh Asoudeh, Nicole Nguyen,* ***Paul Dalhaimer***

8:36 Paper 595c: *Membrane Protein Cryo-EM and Assays in Dynamically Loadable Intact Lipid Bilayers on Nanoporous Membranes* — ***Malcolm Lane Gilchrist***, *Yueming Li*

8:54 Paper 595d: Recombinant Protein Nanostructures for the Inhibition of Sars-Cov-2 — ***Rajarshi Chattaraj***, *Christina Kim, Daeyeon Lee, Daniel A. Hammer*

9:12 Paper 595e: Characterizing Enzyme Cooperativity with Imaging Samdi-MS — ***Blaise Kimmel***, *Jennifer Grant, Milan Mrksich*

9:30 Paper 595f: Delivery and Actuation of Aerosolized Microbots — ***Coy Zimmermann***, *Tyler Schraeder, Brandon Reynolds, Emily DeBoer, Keith B. Neeves, David W. M. Marr*

9:48 Paper 595g: Characterizing Sugar Transporters with Biosensors and Cheminformatics — ***Lily Cheung***

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(596) Molecular and Cellular Sensing Technologies

Thursday, Nov 17, 8:00 AM
Phoenix Convention Center, N-125B

Shachi Mittal, Chair
Qing Sun, Co-Chair
Piyush Jain, Co-Chair

Sponsored by: Bioengineering

8:00 Paper 596a: Image Processing and Immunofluorescent Cell Imaging: Current Challenges and Opportunities — ***Hawley Helmbrecht***, *Elizabeth Nance*

8:18: Break

8:36 Paper 596c: Amplification-Free, Nucleic Acid-Based Detection of Pathogens Using the Lateral Flow Assay Format — *Yan Cao, Zhenrong Zheng, Sukantha Chandrasekaran, Jacob Schmidt, Omai Garner,* ***Harold Monbouquette***

8:54 Paper 596d: Enriching the Cell-Free System Based Biosensor Toolbox to Increase Dynamic Range While Retaining Accuracy — ***Yongchan Kwon***, *Caroline Copeland, Chloe Heitmeier*

9:12 Paper 596e: Small Molecule Detection Using Floating Gate Transistor Biosensors — ***Demetra Adrahtas***, *Jiayi He, Clarice Froehlich, Kaitlyn Gruber, Christy L. Haynes, Kevin Dorfman, C. Daniel Frisbie*

9:30 Paper 596f: A Novel Inductively Coupled Capacitor Wireless Sensor System for Rapid Detection of Bacterial Growth and Antibiotic Susceptibility — ***Yikang Xu***, *Dacheng Ren*

9:48 Paper 596g: Eavesdropping on Neuronal Chemical Chatter Using Optical Sensors Developed from Bio-Conjugated Single Wall Carbon Nanotubes — *Chandima Bulumulla, Andrew Krasley,* ***Abraham Beyene***

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(597) Systems Biology for Engineering Microbes

Thursday, Nov 17, 8:00 AM
Phoenix Convention Center, N-126B

Gregory Reeves, Chair
Jason E. Shoemaker, Co-Chair
Whitney Stoppel, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

8:00 Paper 597a: Roughening Instability of Growing 3D Bacterial Colonies — *Alejandro Martinez-Calvo, Tapomoy Bhattacharjee, R. Konane Bay, Anna Hancock, Ned Wingreen,* ***Sujit Datta***

8:18 Paper 597b: The Instabilities in Bacterial Colony Patterns — ***Uttam Kumar***, *Subramaniam Pushpavanam*

8:36 Paper 597c: Multi-Scale Modeling of Mucin-Driven Modulations of Microbial Phenotypes — ***Mohammad Mazharul Islam***, *Tracy Kuper, Glynis Kolling, Roseanne Ford, Jason A. Papin*

8:54 Paper 597d: Data-Informed Catastrophic and Harmonious Genetic Codon Bias for Multi-Gene Expression — ***Aaron Love***, *Nikhil Nair*

9:12 Paper 597e: High-Throughput Screening of a Promoter Library Reveals New Persister Mechanisms in *Escherichia coli* — ***Sayed Golam Mohiuddin***, *Aslan Massahi, Mehmet Orman*

9:30 Paper 597f: Modeling Temporal Proteome Allocation in Cyanothece Sp. ATCC 51142 Using Prba — ***Kevin Glass***, *Debolina Sakar, Deepro Banerjee, Anindita Bandyopadhyay, Himadri B. Pakrasi, Costas D. Maranas*

9:48 Paper 597g: Invited Talk: Placeholder for the Systems Biology for Engineering Microbes Invited Talk — ***Whitney Stoppel***, *Jason E. Shoemaker, Gregory Reeves*

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(598) Thermochemical Conversion of Biomass

Thursday, Nov 17, 8:00 AM
Phoenix Convention Center, N-228A

Justinus Satrio, Chair
Sunkyu Park, Co-Chair

Sponsored by: Forest and Plant Bioproducts Division

8:00 Paper 598a: Utilization of Marine Macroalgae for the Production of Biofuels and Biomaterials Via Hydrothermal Pyrolysis Process — ***Justinus Satrio***, *Apip Amrullah, Obie Farobie, Michael Berzolla, Hamed Bazrafshan*

8:15 Paper 598b: Pressurized Steam Gasification of Biomass Char – Influence of Temperature and Gas Composition — ***Jieun Kim***, *Kevin Whitty*

8:30 Paper 598c: Surfactant Assisted Hydrothermal Liquefaction of Corn Stover — ***Bharathkiran Maddipudi***, *Khang Huynh, Paiton Mueller, Rajesh Shende*

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(599) Unconventional Oil and Natural Gas: Science & Technology Advancement

Thursday, Nov 17, 8:00 AM
Phoenix Convention Center, W-103A

John McLennan, Chair
Palash Panja, Co-Chair

Sponsored by: Fuels and Petrochemicals Division

8:00 Paper 599a: Solutions of Nonionic Surfactants in CO_2 to Improve Unconventional CO_2-EOR Via Wettability Alteration — *Lauren Burrows, Foad Haeri, Deepak Tapriyal, Sean Sanguinito, Parth Shah, Peter Lemaire III,* ***Robert M. Enick***, *Dustin Crandall, Angela Goodman*

8:15 Paper 599b: Methane Gas Hydrate Formation Kinetics in the Presence of Synthesized Mild and Biodegradable Surfactant — ***Dhaval Patel***, *Bhavikkumar Mahant, Omkar Kushwaha, Rajnish Kumar*

8:30 Paper 599c: Integrated Geochemistry-Geomechanics Approach to Optimization of Hydraulic Fractures Permeability in Caney Shale, SW Oklahoma — *Fengyang Xiong, Connor Allen, Allan Katende, Gabriel Awejori, Brian Kilian, Cody Massion,* ***Mileva Radonjic***

8:45 Paper 599d: A Generalized Druckr-Prager Criterion Modeling for Rock Damage Evolution in Unconvenient Reservoir Underground Circumstance — ***Zongyuan Yao Yao Sr.***

9:00 Paper 599e: Production Performance of US Oil Shale Plays Related to Their Depth Profile and Initial Gas Oil Ratio (GOR) — *Rasoul Sorkhabi,* ***Palash Panja***

9:15 Paper 599f: A Study of Capillary Condensation Phenomena in Mesoporous Materials — ***Jiyue Wu***, *Sheng Hu, Kristian Jessen, Theodore Tsotsis*

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(600) Biomaterials for Drug Delivery II: Hydrogels and Macroscopic Platforms

Thursday, Nov 17, 8:00 AM
Phoenix Convention Center, N-122B

Jennifer Weiser, Chair
Lisa Volpatti, Co-Chair
Yichun Wang, Co-Chair
Rong Tong, Co-Chair

Sponsored by: Biomaterials

8:00 Paper 600a: Implantable Optical Fibers for Immunotherapeutics Delivery and Tumor Impedance Measurement — ***Rong Tong***

8:15 Paper 600b: 4D Printable Salicylic Acid Photopolymers for Sustained Drug-Releasing, Shape Memory Soft Tissue Scaffolds — ***Andrew Weems***

8:30 Paper 600c: Hydrogel Delivery of Statin-Eluting Nanoparticles for Myocardial Infarction Therapy — ***Renato Navarro***, *Narelli Paiva, Sarah C. Heilshorn*

8:45 Paper 600d: Glucose-Fueled Peptide Self-Assembly for Hypoglycemia Rescue — ***Sihan Yu***, *Sijie Xian, Zhou Ye, Irawan Pramudya, Matthew Webber*

9:00 Paper 600e: Tunable Brush-like Polymers on Biomaterials for Controlled Drug Delivery — ***Sanyukta Patil***, *Christopher Foster, Courtney Rowe, Kelly Burke*

9:15 Paper 600f: Liposome-Containing Polyethylene Glycol Microgels for Multi-Therapeutic Delivery — ***Luisa Palmese***, *Paige LeValley, Yingkai Liang, April Kloxin, Kristi L. Kiick*

9:30 Paper 600g: Controlled Release of Growth Factors for Bone Regeneration from Two-Phase Hydrogel Systems — ***Mariya Shevchuk***, *Ryan Reinhart, Nicholas Peppas*

9:45 Paper 600h: Modulating DNA Nanoarchitectures As a Novel, Biomimetic Method of Controlled Therapeutic Release — ***Robert J. Mosley***, *Jacek Wower, Mark Byrne*

(601) Hydrogel Biomaterials I: Emerging Applications

Thursday, Nov 17, 8:00 AM
Phoenix Convention Center, N-121B

Amir Sheikhi, Chair
Marjan Rafat, Co-Chair
Mai Ngo, Co-Chair
Mark Tibbitt, Co-Chair

Sponsored by: Biomaterials

8:00 Paper 601a: Polymer Platforms for 3D Printing Engineered Living Materials — ***Alshakim Nelson***

8:36: Break

8:54 Paper 601c: *Glucose-Responsive Supramolecular Hydrogels* — ***Matthew Webber***

9:12 Paper 601d: Development and Optimization of Poly(vinyl) Alcohol-Alginate Hydrogel Beads for Immobilization of *Rhodococcus Rhodochrous* ATCC 21198 and Slow-Release Compounds — ***Conor Harris***, *Hannah Gedde, Lew Semprini, Skip Rochefort, Kaitlin Fogg*

9:30 Paper 601e: Elucidating the Impact of Lignin Molecular Weight and Composition on the Network Structure and Transport Properties of Lignin-Based Hydrogels for Sustainable Technologies — ***Keturah Bethel***, *Annie Buck, Madeline McCarthy, Xiaoming Lu, Graham W. Tindall, Mark C. Thies, Marc R. Birtwistle, Eric M. Davis*

9:48 Paper 601f: Viral Particle Release from Smart Hydrogel Scaffolds — ***Jorge Leganes Sr.***, *Nicole Steinmetz Sr.*

10:06 Paper 601g: In Vitro Biologics Recovery Tissue Platform with Collagen and Crosslinking Hyaluronic Acid Hydrogels — ***Jessica Torres***, *Fanfei Meng, Kevin Buno, Sathvik Madduri, Paulina Babiak, Luis Solorio, Yoon Yeo, Julie C. Liu*

(602) MOF, COF and Porous Polymer Materials

Thursday, Nov 17, 8:00 AM
Phoenix Convention Center, N-122A

Satish Nune, Chair
Ravichandar Baburao, Co-Chair
Aseem Chawla, Co-Chair

Sponsored by: Inorganic Materials

8:00: Break

8:15 Paper 602b: Bottom-up Vapor-Phase Synthesis of Porphyrin-Based Covalent Organic Frameworks — ***Syed Ibrahim Gnani Peer Mohamed***, *Mona Bavarian, Siamak Nejati*

8:30 Paper 602c: One-Pot Synthesis of Ionic Covalent Organic Frameworks Via Menshutkin Reaction — ***Syed Ibrahim Gnani Peer Mohamed***, *Tan Zhang, Zhen Jiang, Andrew M. Rappe, Siamak Nejati*

8:45 Paper 602d: A Microkinetic Model for Understanding the Synthesis of Thin Film Metal Organic Framework Using Solution Shearing Based Evaporative Crystallization — ***Prem Podupu***, *Prince Verma, Anish Dighe, Rajan Bhawnani, Gaurav Giri, Meenesh Singh*

9:00 Paper 602e: Graphimine - A New Imine-Linked, Two-Dimensional Covalent Organic Framework — ***Kätchen K. Lachmayr***, *Robert H. Lambeth, David C. McLeod, Eric D. Wetzel,* ***Steven Lustig***

9:15 Paper 602f: A Generalizable Approach to Synthesize Polymer-Metal-Organic Framework Gels for Drug Delivery — ***Prince Verma***, *Mara Kuenen, Mark Bannon, Gaurav Giri, Rachel Letteri*

9:30 Paper 602g: Synthesis and Characterization of Two-Dimensional Zeolitic Imidazolate Framework Films — *Qi Liu, Yurun Miao, Michael Tsapatsis,* ***Kumar Varoon Agrawal***

9:45 Paper 602h: Structural Change of ZIF-7: Driven By Either Adsorption or Entropy for CO2 or Bio-Alcohol Separation — ***Yi Du***, *Bradley Wooler, Peter Ravikovitch, Simon C. Weston, Kanmi Mao*

10:00 Paper 602i: Post-Synthetic Modification of Hierarchical Branched ZIF Materials — ***Stephen DeWitt***, *Mostafa Lotfy, Zachary Smith*

(603) Multifunctional Composites

Thursday, Nov 17, 8:00 AM
Phoenix Convention Center, N-121A

Mohammad Hassan, Chair
Elizabeth Bury, Co-Chair
Agoston Kiss, Co-Chair

Sponsored by: Composites

8:00 Paper 603a: Development of a Graphene Oxide Based Composite to Express Multifunctionality of Interest for Aviation Industries. — ***Markus Dieter Ostermann***, *Pierluigi Bilotto, Markus Valtiner*

8:20 Paper 603b: Liquid Metal Multi-Material Dielectric Composites for Multimodal, Deformable Capacitive Pressure Sensing — ***Elizabeth Bury***, *Amanda Koh*

8:40 Paper 603c: Thermomechanical Behavior of Poly(vinyl alcohol)/Graphene Nanoplate (GNP) Composite Films for High-Velocity Impact Applications — ***Mohammad Mansourian-Tabaei***, *Grace Rushing, Rami Al-Sughayer, Hunain Alkhateb, Ahmed Al-Ostaz,* ***Sasan Nouranian***

9:00 Paper 603d: Switchable Crude Oil/Water Nanomulsions Stabilized By Sdbs for Oilfield Applications — *Mohammed Alsakkaf,* ***Sagheer Onaizi***

9:20: Break

9:30 Paper 603e: Hydrothermal Synthesis of Titanium Dioxide-Graphene Oxide Quantum Dots (TiO_2-GOQDs) Nanocomposites for Enhanced Photocatalytic Activity — ***Fahmi Asyadi Md Yusof***, *Zulhafiz Tajudin*

9:50 Paper 603f: BN/TiO_2 Nanocomposite for Photocatalytic Phenol Degradation — ***Aboubakr Abdullah***

10:10 Paper 603g: Effect of H_2 Reduction and Ferrocene Role in the Production Lengthy CNT Bundles — ***Zuhayr Malaibary***

(604) Polymer Viscoelasticity: Mechanics, Processing, and Rheology I

Thursday, Nov 17, 8:00 AM
Phoenix Convention Center, N-121C

Gregory McKenna, Chair
Nader Taheri-Qazvini, Co-Chair
Amanda Marciel, Co-Chair
Sara Hashmi, Co-Chair

Sponsored by: Polymers

8:00 Paper 604a: Rheology, Processing and Mechanical Properties of Carbon Fiber Precursor Polymer — *Ning Bian, Samsuddin Mahmood, Rajat Srivastava, Ashutosh Shrivastava, Duck Yang,* ***Hongbing Lu***

8:30 Paper 604b: Liquid Shear-Based Nanofabrication Technique As a Tool for Producing a Plethora of Soft Polymeric Morphologies — ***Rachel Bang***, *Sangchul Roh, Austin Williams, Orlin D. Velev*

8:45 Paper 604c: Dynamic Associations Facilitate Macromolecular Engineering of Formulations — ***Carina Martinez***, *Vivek Sharma*

9:00 Paper 604d: Temperature-Controlled Dripping-Onto-Substrate (DoS) Extensional Rheometry of Polymer Micelle Solutions — *Diana Y. Zhang,* ***Michelle Calabrese***

9:15 Paper 604e: Rheological Models for Wormlike Micelles: Advances, Limitations, and Promising Future Directions — ***Joseph Peterson***, *Weizhong Zou*

9:30 Paper 604f: Characterization of As-Prepared Polymeric Films By Simultaneously Measuring the Glass Transition, Crystallinity, and Order-Disorder Transition through the Restitution — ***Jinwon Park***, *Seongsoo Han, Hyeonjung Park, Jaehong Lee, Suchan Cho, Myungeun Seo, Bumjoon J. Kim, Siyoung Q. Choi*

9:45 Paper 604i: Rheology-Manipulated Feedstocks for in-Line Sublayers in a New 3D Printing Mechanism — ***Dharneedar Ravichandran***, *Kenan Song*

10:00 Paper 604j: Tailoring Liquid Crystal Elastomer Networks for Shape Programming and Additive Manufacturing — *Morgan Barnes, Seyed M. Sajadi, Shaan Parekh, Muhammad Rahman, Pulickel M. Ajayan,* ***Rafael Verduzco***

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(605) Advances in New Modalities: Peptides, Nucleic acids

Thursday, Nov 17, 8:00 AM
Phoenix Convention Center, N-123

Christopher Lowe, Chair
Steve Rhieu, Co-Chair
Satheesh Podaralla, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

8:00 Paper 605a: Scaleup Considerations for Solid-Phase Peptide Synthesis in Highly Dynamic Packed Beds. — ***Harrison Rose***, *Mike Di Maso, Kyle E. Ruhl, Shane T. Grosser, François Lévesque, Kevin M. Maloney, U. Faruk Mansoor, Ritwika Ray, Danielle M. Schultz, Steven M. Silverman*

8:24 Paper 605b: New Insights into the Difficulties and Importance of Dichloroacetic Acid Removal Post Detritylation in the Solid Phase Oligonucleotides Synthesis Cycle — ***Peng-Kai Kao***, *Todd Kajdan, Timothy M. Braden, Chen-Chun Chen, David Logsdon, Wei-Ming Sun, Eric D. Moher, Martin Johnson, Yufei Wei*

8:48 Paper 605c: Process Bottleneck of Packed Bed Oligonucleotide Reactors Arising from Critical Flux Due to Solid Phase Compressibility — ***Yufei Wei***, *Al Khilevich, Wei-Ming Sun, Martin Johnson, Timothy M. Braden, Chen-Chun Chen*

9:12 Paper 605d: Study of Factors Impacting Peptide Retention in Nanofiltration — ***Paridhi Agrawal***, *Kevin D. Seibert*

9:36 Paper 605e: Digital Process Replica of RNA Manufacturing for Enabling Process Optimization, Technology Transfer and Techno-Economic Assessment — ***Simon Daniel***, *Zoltán Kis, Cleo Kontoravdi, Nilay Shah*

10:00 Paper 605f: A 3D-Printed Microfluidic Device for High-Throughput Production of mRNA-Lipid Nanoparticles — ***Wan-Zhen Lin***, *Kristian Bostic, Noah Malmstadt*

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(606) Computational Solid State Pharmaceutics I

Thursday, Nov 17, 8:00 AM
Phoenix Convention Center, N-122C

Yuriy Abramov, Chair
Ebenezer Ojo, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

8:00 Paper 606a: The Importance of Solid-State Modeling in Drug Development — ***Luca Iuzzolino***

8:25 Paper 606b: Identifying and Addressing the Weaknesses of Density Functional Theory for Crystal Structure Prediction — ***Gregory Beran***

8:50 Paper 606c: Rational Reduction of Computationally Predicted Crystal Energy Landscapes Using Molecular Dynamics and Enhanced Sampling Techniques. — *Nicholas F. Francia, Louise Price, Sally L. Price,* ***Matteo Salvalaglio***

9:15 Paper 606e: A Novel Computational Approach to Guide Impurities Rejection By Crystallization — ***Yuriy Abramov***, *Amanuel Zelellow, Michal Achmatowicz, Cheng Chen, Jian Wang, Sivakumar Sekharan, Michael A. Bellucci*

9:40 Paper 606f: Polymorphism in a Lennard-Jones Fluid Nucleating from Its Melt — ***Pelin Su Bulutoglu***, *Shiyan Wang, Nandkishor Nere, Doraiswami Ramkrishna*

10:05 Paper 606g: Assessment of Force Fields for Crystal Morphology Prediction — ***Yongsheng Zhao***, *Robert Gee, Michael F. Doherty*

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

Thursday, Nov 17, 8:00 AM
Phoenix Convention Center, N-221C

Hee Jeung Oh, Chair
Christine Duval, Co-Chair

Sponsored by: Membrane-Based Separations

8:00 Paper 607a: Novel Polyether-Based Amphoteric Ion Exchange Membrane for Electrochemical Systems — ***Gouree Kumbhar***, *Geetanjali Shukla, Robert C. Ferrier Jr., Caroline Szczepanski, David Hickey, Chase Bruggeman*

8:21 Paper 607b: Synthesis and Performance Characterization of Zwitterionic Poly(arylene ether sulfone) Copolymers for Fouling-Resistant Desalination Membranes — *Matthew D. Green,* ***Husain Mithaiwala***

8:42 Paper 607c: Co-Transport of Lithium, Sodium, and Potassium Ions in Pegylated Sulfonated Polysulfones — ***Jung Min Kim***, *Sean Bannon, Patrick M. McCormack, Geoffrey Geise*

9:03 Paper 607d: A Novel Solar Energy Driven Photoelectrodialysis Approach for Brackish Water Desalination — ***Syed Islam***, *Jackie Zheng, Nadeesha Lakmali Kothalawala, Prakhar Sharma, Ilia N. Ivanov, Ramesh Bhave, Doo Young Kim, Tomonori Saito, Priyesh Wagh*

9:24 Paper 607e: Obtaining Structure-Function Insight from High-Throughput Membrane Characterization — ***Jonathan Ouimet***, *Laurianne Lair, Xinhong Liu, Elvis Eugene, Alexander Dowling, William Phillip*

9:45 Paper 607f: Separation of Urea from Water Solution Using Sulfonated Poly (styrene-isobutylene-styrene) Membranes with Counter-Ion Substitution — ***Juan Rivera-Diaz***, *David Suleiman*

10:06 Paper 607g: Stripping of Metal Ions for Ionic Liquid Recycling in a Self-Optimizing, Continuous Process — ***Bin Pan***, *Lanja R. Karadaghi, Richard L. Brutchey, Noah Malmstadt*

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(608) Experimental Methods in Adsorption

Thursday, Nov 17, 8:00 AM
Phoenix Convention Center, N-130

Sasidhar Gumma, Chair
Enzo Mangano, Co-Chair

Sponsored by: Adsorption and Ion Exchange

8:00 Paper 608a: Determining CO_2/H_2S and CO_2/CH_4 Binary Adsorption Selectivities in Metal-Organic Frameworks for Biogas Purification — ***Chunyi Li***, *Ryan P. Lively*

8:25 Paper 608b: Diffusion of CO_2 and N_2 in 5A Pellets Measured Using the Adsorption Differential Volumetric Apparatus — *JinYu Wang, Enzo Mangano, Stefano Brandani,* ***Federico Brandani***, *Pluton Pullumbi*

8:50: Break

9:15 Paper 608d: Miniaturizing Dynamic Column Breakthrough Measurements to Measure Gas and Vapour Adsorption Equilibrium on Milligram Quantities of Adsorbents — ***Nicholas Wilkins***, *James Sawada, Noelie Consant, Arvind Rajendran*

9:40 Paper 608e: Direct Measurement of the Mass Transport Coefficient of Water in Silica-Gel Using the ZLC Technique — ***Stefano Brandani***, *Enzo Mangano*

10:05 Paper 608f: Binary Adsorption of CO_2 and H_2o on Uio-66 and Amine-Functionalized Uio-66 Metal-Organic Frameworks — *Arianjel Hernandez, Rebekah K. Impastato, Mohammad I. Hossain, Brooks Rabideau,* ***T. Grant Glover***

(609) Membrane Formation

Thursday, Nov 17, 8:00 AM
Phoenix Convention Center, N-132A

Ali Rownaghi, Chair

Sponsored by: Membrane-Based Separations

8:00 Paper 609a: Preparation of Polyethersulfone Membranes on Non-Woven Fabric Supports — ***Joseph Danner***, *Blake Jarrell, Steven Weinman*

8:21 Paper 609b: Pervaporative Alcohol Dehydration Using PVA-TEOS-CMS Hybrid Membrane — ***Musabbir Jahan Talukder***, *Ali Alshami*

8:42 Paper 609c: Tunable Amphiphilic Pdmaema-b-PS Block Copolymer and Ionic Liquid Composite Thin Films for Gas Separations — ***Charlie Knight***, *Paul Scovazzo, Sasan Nouranian, Adam Smith, Alexander Lopez*

9:03 Paper 609d: Ultrasonicated *in Situ* Growth of Ag-MOF in Polyamide Selective Layer of Thin Film Nanocomposite Membranes: Fabrication, Characterization, and Performance — ***Medha Kasula***, *Milad Esfahani*

9:24 Paper 609e: High Flux Porous Structure Formation in Isoporous Thin Film Membranes through Selective Domain Assembly — ***Khadar Shaik***, *Ali Ammar, Kshitij Sharma, Diana Cousins, Maninderjeet Singh, Deepalekshmi Ponnamma, Mohammad Hassan, Samer Adham, Mariam Al-Maadeed, Anil Bhowmick, Alamgir Karim*

9:45 Paper 609f: Fabricating a 'Breathable' Porous Flat Sheet Membrane Via Non Solvent Induced Phase Separation (NIPS) for Face Masks and Other Air Filtration Applications — ***Ebuka Ogbuoji***, *Isabel Escobar*

10:06 Paper 609g: Formation of Hydrogen-Selective Carbon Composite Membranes By Incomplete Stabilization of Polyacrylonitrile — ***H. Enis Karahan***, *Wataru Nakata, Behnam Ghalei*

(610) Molecular and Data Science Modeling of Adsorption II

Thursday, Nov 17, 8:00 AM
Phoenix Convention Center, N-131C

Peter Ravikovitch, Chair
Alexander Neimark, Co-Chair
Gennady Gor, Co-Chair

Sponsored by: Adsorption and Ion Exchange

8:00 Paper 610a: Selective Removal of Selenate from Selenate-Sulphate Water Solution By Adsorption on Dispersed Single Atoms on [012] Al_2O_3 Surface: An Ab-Initio Study — ***Srishti Gupta***, *Adam Chismar, Christopher Muhich*

8:15 Paper 610b: Modeling the Interactions of Heavy Organic Aerosols with Water-Harvesting Metal-Organic Frameworks — ***Raghuram Thyagarajan***, *David Sholl*

8:30 Paper 610c: Predicting Adsorption of 1,4-Dioxane in All-Silica Zeolites Using Molecular Simulations — ***Samiha Sharlin***, *Tyler R. Josephson*

8:45 Paper 610d: Accelerating Solvent Selection for Type II Porous Liquids — ***Chao-Wen Chang***, *Isaiah Borne, Robin Lawler, Ryan P. Lively, David Sholl*

9:00 Paper 610e: Computational Investigation of Mxene Family for Different CO_2/H_2 Mixture Adsorption Processes: VSA, PSA, TSA, Ptsa, and Vtsa — ***Melih Doganci***, *Sadiye Velioglu*

9:15 Paper 610f: Quantitative Insights into the Influence of MOF Defects on Adsorption Properties — ***Zhenzi Yu***, *Cai Xuqing, David Sholl*

9:30 Paper 610g: A Molecular-Scale Study of Monazite Beneficiation through Computational and Spectroscopic Techniques — ***Luke Gibson***, *Diana Stamberga, Vera Bocharova, Benjamin Doughty, Robert Sacci, Lawrence Anovitz, Vyacheslav S. Bryantsev*

9:45 Paper 610h: Implementation of Genetic Algorithms to Optimize Metal-Organic Frameworks for CO_2 Capture — ***Thang Pham***, *Randall Snurr*

10:00 Paper 610i: Prediction of Metal-Organic Interactions and Molecular Assembly in High Accuracy and Speed — ***Cheng Zhu***, *Samuel Edmund Hoff, Hendrik Heinz*

(611) Solid Form Selection: Cocrystals, Salts, Solvates, Polymorphs, and Beyond

Thursday, Nov 17, 8:00 AM
Phoenix Convention Center, N-131A

Haitao Zhang, Chair
Mo Jiang, Co-Chair
Daniel Green, Co-Chair

Sponsored by: Crystallization and Evaporation

8:00: Welcoming Remarks

8:03 Paper 611a: Role of Solid Solutions in Polymorphic Enantiotropy — ***Fredrik Nordstrom***, *Brian Linehan, Francesco Ricci*

9:01: Concluding Remarks

(612) Transformation from Batch to Continuous Processing in Bioseparations

Thursday, Nov 17, 8:00 AM
Phoenix Convention Center, N-131B

Caryn Heldt, Chair
Maximilian Wessner, Co-Chair

Sponsored by: Bio Separations

8:00 Paper 612a: The iSKID Platform: At the Crossroads of Technical Development and Manufacturing Readiness — ***Jeff Salm***

8:40 Paper 612b: Continuous Purification of a Viral Vaccine Using Aqueous Two-Phase Extraction and Tangential Flow Filtration — ***Natalie Nold***, *Sheridan Waldack, Grace James, Trisha Colling, Seth Kriz, Caryn Heldt*

9:00 Paper 612c: A Tubular Membrane-in-a-Shell Microextractor for Continuous Separation of Antibiotic Precursors — ***Michal Pribyl***, *Lukas Sauer, Zdenek Slouka*

9:20 Paper 612d: Effect of Membrane Module Geometry on the Critical Flux for IgG Precipitates — ***Mirko Minervini***, *Andrew Zydney*

9:40 Paper 612e: UV-Vis Spectroscopy-Based PLS Inferential Sensor for Detection of Host Cell Proteins in Concentrated Antibody Solution — ***Ian Gough***, *Claire Velikonja, Brandon Corbett, Thomas Kruse, David Latulippe, Prashant Mhaskar*

10:00 Paper 612f: Continuous Downstream Process of Antibody Developed Based on the Process Analysis and Understanding — *Fuminori Konoike, Noriko Yoshimoto,* ***Shuichi Yamamoto***

(613) Advances in Life Cycle Assessment

Thursday, Nov 17, 8:00 AM
Phoenix Convention Center, N-226A

Tapajyoti Ghosh, Chair
Bhavik Bakshi, Co-Chair
Vikas Khanna, Co-Chair

Sponsored by: Sustainability Science and Engineering

8:00 Paper 613a: Technology Assessment and Impact Analysis for Life Cycle Based Sustainability Performance Improvement of Process Systems — ***Abdurrafay Siddiqui***, *Yinlun Huang*

8:20 Paper 613e: Building a prospective LCA framework to analyze emerging technologies in a dynamic system context — ***Tapajyoti Ghosh***, *Patrick Lamers, Alberta Carpenter*

8:40 Paper 613c: Encouraging 'Nature Positive' Decisions: Toward an Open-Source Tool for Ecosystem Services-Based Absolute Environmental Sustainability Assessment — ***Ying Xue***, *Bhavik Bakshi*

9:00 Paper 613d: Circular Economy Approach in the Valorization of Rare Earths Generated in Alluvial Mining By Quantifying Environmental Impacts through Life Cycle Analysis — ***Natalia Cano***, *Sebastián Barrientos-Benjumea, Luz Marina Ocampo, Jo Dewulf*

(614) Biological Conversions and Processes for Renewable Feedstocks

Thursday, Nov 17, 8:00 AM
Phoenix Convention Center, N-226B

Rebecca Ong, Chair
Shishir Chundawat, Co-Chair
Hasan Atiyeh, Co-Chair

Sponsored by: Sustainable Biorefineries

8:00 Paper 614a: Conversion of CO_2 into C2-C6 Products By *Clostridium Muellerianum* Sp. Nov. Strain P21 — *Rahul Thunuguntla,* ***Hasan Atiyeh***, *Raymond L. Huhnke, Ralph S. Tanner*

8:15 Paper 614b: Biocatalytic Production of Biomass-Based Chemical Derivatives — ***Victor Sharma***, *Vyoma Maroo, Thomas Binder, Kyle Camarda, Alan Allgeier, Jeffrey McFarlane, Kylee Cosse*

8:30 Paper 614c: Novel Enzymatic Treatment to Enhance Delamination of Corn Stalk for Efficient Separation of Pith and Rind — ***Asif Hasan Rony***, *Bradley Wahlen, Lynn Wendt, William A. Smith*

8:45 Paper 614d: A Novel Phenotype of Haloalkaliphilic Methanotrophs Induced By Extreme Oxidative Stress — ***Alisabeth Bradford***, *Kiumars Badr, Marina G. Kalyuzhnaya, Q. Peter He, Jin Wang*

9:00 Paper 614e: In-Situ Bio-Electrochemical Sulfide Remediation during the Storage and Anaerobic Digestion of Dairy Manure — ***Lingkan Ding***, *Bo Hu*

9:15 Paper 614f: A Genome Scale Model for Prediction of Growth Rates and Fluxes for *Rhodococcus Opacus* PD630 Metabolism — ***Garrett W. Roell***, *Christina Schenk, Winston Anthony, Rhiannon Carr, Gautam Dantas, Yinjie Tang, Tae Seok Moon, Hector Garcia Martin*

9:30 Paper 614g: Antibacterial Activity of AGRO-Industrial Wastes and Common Plants Extracts for Health and Industrial Applications – Towards Circular Bioeconomy and Sustainability — ***Lourdes Orejuela Escobar***, *Arleth Gualle Brito, Andrés Lagos, Andrea Landázuri, Jose Miguel Alvarez Suarez, Miguel Angel Mendez, Daniel Aguilera-Pesantez, Patricio Rojas*

(615) Policy and Sustainability

Thursday, Nov 17, 8:00 AM
Phoenix Convention Center, N-226C

Ashley Pennington, Chair
Jason Trembly, Co-Chair
Gerardo Ruiz-Mercado, Co-Chair

Sponsored by: Sustainable Energy

8:00 Paper 615a: Environmental Release and Occupation Exposure Models Used in Chemical Risk Evaluation — ***William Barrett***

(616) Engineering Cancer III: Devices for Diagnosis, Culturing, and Microenvironment Studies

Thursday, Nov 17, 8:00 AM
Phoenix Convention Center, N-126C

Swomitra Mohanty, Chair
Rick Liao, Co-Chair

Sponsored by: Chemical Engineers in Medicine

8:00 Paper 616a: Nature-Inspired 3D Scaffolds to Improve *Ex Vivo* T-Cell Culturing Environments for Adoptive Cell Transfer Cancer Immunotherapy — ***Lucy Todd***, *Matthew Chin, Marc-Olivier Coppens*

8:18 Paper 616b: Isolation and Identification of Subpopulations of Circulating Tumor Cells Using a Microchip with Bio-Inspired Patterns — ***Wei Li***, *Zhenya Ding*

8:36 Paper 616c: Dynamic 3D Co-Culture of Stromal and Immune Cells with ER^+ Breast Cancer Using a Thiol-Acrylate Hydrogel Scaffold and Microfluidic Droplet Trapping Array — ***Braulio Ortega Quesada***, *Anowar H. Khan, Sophia Zhou, Elizabeth C. Martin, John Pojman, Adam Melvin*

8:54 Paper 616d: Cell-Free Protein Synthesis Biosensing of Glutamine in Human Serum and Saliva: Towards at-Home Low-Cost Diagnostics for Personalized Cancer Treatment — ***Brad Bundy***, *J Porter Hunt, Mehran Soltani*

9:12 Paper 616e: Investigating Intracellular Adhesion and Intercellular Signaling in Glioblastoma Models — ***Rosalyn Hatlen***, *Padmavathy Rajagopalan*

9:30 Paper 616f: Probing the Spatiotemporal Attributes of Gamma-Secretase/Notch Signaling in Breast Cancer Microenvironments — ***Malcolm Lane Gilchrist***, *Yueming Li*

9:48 Paper 616g: Multivariate Model of an Engineered Niche Delineates Metastatic Potential of Breast Cancer — ***Sophia Orbach***, *Christian DeVaull, Elizabeth Bealer, Jacqueline Jeruss, Lonnie Shea*

10:06 Paper 616h: Multimodal Imaging for Simultaneous Measurement of Melanocyte Mass and Pigmentation — ***Tarek Moustafa***, *Edward Polanco, Rachel Belote, Robert Judson-Torres, Thomas Zangle*

(617) Catalysis on Low Dimensional Materials II: Single Atom Catalysts

Thursday, Nov 17, 12:30 PM
Phoenix Convention Center, N-127A

Arthur Shih, Chair
Pushkar Ghanekar, Co-Chair

Sponsored by: Catalysis

12:30 Paper 617a: Ab Initio Study of Organometallic Phthalocyanine Catalysts for the Conversion of Methane to Methanol — ***Chase Ferrone***, *Pabitra Choudhury*

12:48 Paper 617b: Interfacial Potential, Coverage and Solvation Effects on the in-Situ Structure, Stability and Activity of Fe-N-C Catalysts during ORR — ***Ankita Morankar***, *Siddharth Deshpande, Zhenhua Zeng, Alyssa McNarney, Plamen Atanassov, Jeffrey Greeley*

1:06 Paper 617c: Coupling Potential Dependency and Spin Effects in Graphene-Based Single Atom Catalysts for Oxygen Evolution and Reduction Reactions — ***Md Delowar Hossain***, *Michal Bajdich*

1:24 Paper 617d: Formic Acid Electro-Oxidation over Graphene-Based Single Atom Catalysts: A Case Study on Coverage Effects — ***Michael Rebarchik***, *Manos Mavrikakis*

1:42 Paper 617e: Spin-Crossing in Heterogeneous Catalysis By Atomically Dispersed Transition Metals. an Example: Ethane Dehydrogenation By Co/SiO_2 — ***Sanjana Srinivas***, *Stavros Caratzoulas, Dionisios Vlachos*

2:00 Paper 617f: Dynamical Evolution of Atomically Dispersed Precious Metals on Oxide Supports — *Nicholas Humphrey, Selin Bac,* ***Shaama Mallikarjun Sharada***

(618) CO_2 Upgrading I: Thermocatalytic Approaches to the Production of Fuels and Chemicals

Thursday, Nov 17, 12:30 PM
Phoenix Convention Center, N-128A

Carlos Morales-Guio, Chair
Erdem Sasmaz, Co-Chair

Sponsored by: Catalysis

12:30 Paper 618a: X-Ray Absorption Spectroscopy Reveals the Dynamic Nature of Catalysts — ***Aisulu Aitbekova***, *Liheng Wu, Simon Bare, Matteo Cargnello*

12:48 Paper 618b: Understanding CO_2 Conversion to Methanol on $Cu/ZnO/Al_2O_3$ Using Microkinetic Modelling — *Anže Prašnikar, Andraž Pavlišič, Damjan Lašič Jurković, David Bajec, Matic Grom,* ***Blaž Likozar***

1:06 Paper 618c: Catalytic Hydrogenation of CO_2 to Methanol Enabled By the Metal-Lewis Acid Interfaces in Metal-Organic Frameworks (MOFs) Uio-66 — ***Huy Nguyen***, *Jingyun Ye, Donald G. Truhlar, Johannes A. Lercher, Matthew Neurock*

1:24 Paper 618d: Tuning Selectivity of CO_2 Methanation over $MgO-Ni/SiO_2$ — ***Yufei Xie***, *Valentijn De Coster, Hilde Poelman, Vladimir Galvita*

1:42 Paper 618e: Influence of Rhodium Nuclearity Embedded in Metal Oxide Frameworks for CO_2 hydrogenation — ***Shuting Xiang***, *Juan Jimenez, Luisa Posada, Samantha Rubio, Steven L. Suib, Anatoly I. Frenkel, Sanjaya D. Senanayake*

2:00: Break

2:18 Paper 618g: In Situ CO_2 Capture and Catalytic Hydrogenation at Ni/Alkaline Earth Carbonate Interfaces — ***WU Xianyue***, *Wen Liu, Ribooga Chang, Ocean Cheung*

2:36 Paper 618h: Scale up Considerations for CO_2 Direct Air Capture (DAC) and Catalytic Conversion to Renewable Natural Gas Using a Dual Function Material (DFM) Washcoated Monolith — ***Monica Abdallah***, *Robert Farrauto*

(619) Electrocatalysis IV: Modeling, Kinetics, and Characterization

Thursday, Nov 17, 12:30 PM
Phoenix Convention Center, N-127C

Elizabeth Biddinger, Chair
Miguel Modestino, Co-Chair
G. T. Kasun Kalhara Gunasooriya, Co-Chair

Sponsored by: Catalysis

12:30 Paper 619a: DFT Screening of Transition Metal-Doped CdS Catalysts for Green Hydrogen Production By H_2s and H_2o Splitting — ***Yuting Li***, *Daniel Bahamon, Mutasem Sinnokrot,* ***Lourdes Vega***

12:48 Paper 619b: Theoretical Modeling of Interfacial Proton-Coupled Electron Transfer — ***Robert Warburton***, *Phillips Hutchison, Alexander Soudackov, James M. Mayer, Sharon Hammes-Schiffer*

1:06 Paper 619c: Stability of Metal Oxides on Metal Nanoparticles and Its Impact on Oxygen Reduction Reaction. — ***Kaustubh Sawant***, *Zhenhua Zeng, Junxian Gao, Dmitry Zemlyanov, Jeffrey T. Miller, Jeffrey Greeley*

1:24 Paper 619d: Monitoring in Situ Stress Generation on Au Electrocatalyst during Electrochemical Oxygen Evolution and Reduction Reactions for Li-O2 Batteries — *Hannah Dykes, Bertan Ozdogru,* ***Omer Ozgur Capraz***

1:42 Paper 619e: Continuum Modeling of Metal-Insulator-Semiconductor (MIS) Photoelectrodes — ***Alex King***, *Adam Weber, Alexis T. Bell*

2:00 Paper 619f: Probing the Reaction Microenvironment during Electrochemical Nitrate Reduction — ***Elizabeth Corson***, *Jinyu Guo, Matthew Liu, Carolina Munoz, William Tarpeh*

2:18 Paper 619g: *In-Situ* Exsolution of Bimetallic Cofe Nanoparticles on $(La,Sr)FeO_3$ Perovskite: Its Effect on Oxidative Coupling of Methane — ***Jaesung Kim***, *Yu Jin Kim, Matthew Ferree, Seval Gunduz, Anne Co, Minkyu Kim, Umit Ozkan*

2:36 Paper 619h: Controlling the Electrochemical Kinetics of Hydrocarbon Synthesis from CO_2 and the Electrocatalytic Transformation of Ethanol to Ethylene Oxide — ***Marcel Schreier***

(620) Pyrolysis of Biomass

Thursday, Nov 17, 12:30 PM
Phoenix Convention Center, N-128B

Hsu Chiang, Chair
Lucas Ellis, Co-Chair

Sponsored by: Reaction Engineering

12:30 Paper 620a: A Combined Experimental and Modelling Study of Biomass Fast Pyrolysis — ***Falak Naz***, *Nikhil Kumar, Himanshu Goyal, Varunkumar S*

12:50 Paper 620b: Influence of Lignin-Carbohydrate Complex (LCC) Linkages on the Pyrolytic Decomposition of Carbohydrates in Biomass — ***Arul Mozhi Devan Padmanathan***, *Khursheed B. Ansari, Samir H. Mushrif*

1:10 Paper 620c: Mechanistic Insights into the Pyrolysis of Crystalline and Amorphous Celluloses — ***SriBala Gorugantu***, *Diana Vargas, Pavlo Kostetskyy, Ruben Van de Vijver, Linda Broadbelt, Guy Marin, Kevin Van Geem*

1:30 Paper 620d: Optimal Biochar Catalyst Screening for Upgrading Pyrolysis Products — ***Zhongzhe Liu***, *Matthew Hughes, Yiran Tong, Jizhi Zhou, William Kreutter, Hugo Cortes Lopez, Simcha Singer, Daniel Zitomer, Patrick McNamara*

1:50 Paper 620e: Pulse-Heated Pyrolysis of a Model Lignin Tetramer: Experimental and Computational Reaction Insights — ***Ross Houston***, *Nourredine Abdoulmoumine*

2:10 Paper 620f: Evaluation of Pyrolysis Wax As a Solvent in Polyolefin Pyrolysis Processing — ***Ali Zolghadr***, *Daniel Kulas, David Shonnard*

2:30 Paper 620g: Unraveling the Radical Decomposition Chemistry of Longer-Chain Oxymethylene Ethers (OME-4 and OME-5): High-Potential e-Fuels — ***Kevin De Ras***, *Olivier Herbinet, Frédérique Battin-Leclerc, Joris Thybaut, Kevin Van Geem*

(621) Reaction Chemistry & Engineering II

Thursday, Nov 17, 12:30 PM
Phoenix Convention Center, N-127B

Manish Shetty, Chair
Milad Abolhasani, Co-Chair

Sponsored by: Reaction Engineering

12:30 Paper 621a: Flexible Homogeneous Hydroformylation: On-Demand Tuning of Aldehyde Branching with a Cyclic Fluorophosphite Ligand — ***Jeffrey Bennett***, *Malek Y.S. Ibrahim, Milad Abolhasani*

12:48 Paper 621b: Impact of Feed Composition on the Spatial Features of Coupled Methane Oxidation and Reforming — ***Jonathan Ratcliff***, *Kyle Karinshak, Michael Harold*

1:06 Paper 621c: A New Strategy of *in-Situ* Enzyme Immobilization Based on Self-Assembly Hydrogel for Continuous-Flow Biocatalysis for the Synthesis of Chiral Alcohols — ***Qiang Chen***, *Yujun Wang, Guangsheng Luo*

1:24: Break

1:42 Paper 621e: Facile Synthesis of Uniform $Fe_2O_3@Y_2O_3$ Yolk-Shell Oxygen Carriers for Chemical Looping Applications — *Qianwenhao Fan,* ***Wen Liu***

2:00 Paper 621f: Kinetic Study for the Hydrogen Production Via Water-Splitting of Ascorbic Acid with a CdS-ZnS/Pt Binary Photocatalyst — *Tayseir Mohammed,* ***Konstantinos E. Kakosimos***

2:18 Paper 621g: An End-to-End Workflow for Diverse Transition State Conformer Generation Using Machine Learning — *Lagnajit Pattanaik,* ***Xiaorui Dong***, *Haoyang Wu, Kevin Spiekermann, Hao-Wei Pang, William Green*

2:36 Paper 621h: Gas Flow Mapping in Different Sizes Gas-Solid Fluidized Bed Reactors Via Advance Non-Invasive Measurement Techniques* — ***Abdelsalam Efhaima Sr.***, *Al-Dahhan Muthanna Sr., Asfaw Gezae Daful Sr.*

(622) Machine Learning for Soft Materials I

Thursday, Nov 17, 12:30 PM
Phoenix Convention Center, N-222B

Michael Webb, Chair
Nicholas Jackson, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

12:30: Introductory Remarks

12:35 Paper 622a: Inverse Design of Pore Wall Chemistry to Control Solute Transport through Molecular Simulation Coupled Optimization — ***Sally Jiao**, M. Scott Shell*

12:50 Paper 622b: Multi-Multimolecular Latent Space Simulations of DNA Hairpin-Duplex Competition — ***Mike Jones**, Andrew Ferguson*

1:05 Paper 622c: Machine Learning-Enabled Prediction of Electronic Properties of Radical Polymers at Coarse-Grained Resolutions — ***Riccardo Alessandri**, Juan J. de Pablo*

1:20 Paper 622d: Machine Learning Guided Discovery of Polymer Membranes for Reducing Greenhouse Gas Emissions — ***Yasemin Basdogan**, Zhen-Gang Wang*

1:35: Break

2:00 Paper 622e: Sigma Profiles in Deep Learning: Towards a Universal Molecular Descriptor — ***Dinis O. Abranches**, Yong Zhang, Edward Maginn, Yamil Colón*

2:15 Paper 622f: Systematic Investigation of Training Protocols for Machine Learning Derived Interatomic Potentials — ***Nisarg Joshi**, Jim Pfaendtner*

2:30 Paper 622g: Application of Machine Learning to Accelerate High-Throughput Molecular Dynamics Screening: A Study of Tribological Properties of Monolayer Films — ***Co D. Quach**, Justin Gilmer, Daniel Pert, Akanke Mason-Hogans, Peter Cummings, Clare McCabe*

2:45 Paper 622h: Detecting Transition Boundaries in Molecular Simulations — ***Brandon Butler**, Domagoj Fijan, Sharon C. Glotzer*

(623) Modeling, Control, and Optimization of Energy Systems II

Thursday, Nov 17, 12:30 PM
Phoenix Convention Center, W-101B

Yuhe Tian, Chair
Sungho Shin, Co-Chair

Sponsored by: Systems and Process Control

12:30 Paper 623a: Multistage NMPC for Demand Uncertainty of Gas Pipeline Networks — ***Sakshi Naik**, Robert Parker, Michael Bynum, Carl Laird, Lorenz Biegler*

12:49 Paper 623b: Multi-Stage Dynamic Optimization-Based Scheduling & Demand Side Management of Hybrid Renewable Energy Systems Under Uncertainties — ***P S Pravin**, Xiaonan Wang, Zhe Wu*

1:08 Paper 623c: A Two-Level Optimization Framework with Consideration of Economic Benefits and Long-Term Capacity Fading for Battery Energy Storage Systems — ***Jiwei Yao**, Tao Gao, John Hedengren, Kody Powell*

1:27 Paper 623d: Bayesian Optimization with Reference Models: A Case Study in MPC for HVAC Central Plants — ***Qiugang Lu**, Leonardo Gonzalez, Ranjeet Kumar, Victor Zavala*

1:46 Paper 623e: Nonlinear Model Predictive Control for Power Plant Steam Cycles with Online Model Re-Identification — ***Daniel Kestering**, Victor Alves, Selorme Agbleze, Fernando V. Lima*

2:05 Paper 623f: Autoencoder Based Dimensionality Reduction to Select Representative Periods for Energy System Planning Models — *Marc Barbar, **Dharik Mallapragada***

2:24 Paper 623g: Technoeconomic Assessment of Coupling an Existing Nuclear Power Plant with a Low Temperature Electrolysis Unit — ***Radhakrishna Tumbalam Gooty**, Konor Frick, Jaffer Ghouse, Jason Hansen, John Siirola, David Miller*

2:43 Paper 623h: Multiscale Computational Fluid Dynamics Modeling of Spatial Atomic Layer Etching for Aluminum Oxide Thin Films — ***Sungil Yun**, Matthew Tom, Feiyang Ou, Henrik Wang, Gerassimos Orkoulas, Panagiotis Christofides*

(624) Data-driven optimization

Thursday, Nov 17, 12:30 PM
Phoenix Convention Center, W-101A

Matthew Stuber, Chair
Burcu Beykal, Co-Chair

Sponsored by: Information Management and Intelligent Systems

12:30 Paper 624a: Branch-and-Model: A Derivative-Free Global Optimization Algorithm — ***Kaiwen Ma**, Luis Miguel Rios, Atharv Bhosekar, Nikolaos Sahinidis, Sreekanth Rajagopalan*

12:49 Paper 624b: Data-Driven Coordination in Enterprise-Wide Optimization — ***Damien van de Berg**, Panagiotis Petsagkourakis, Nilay Shah, Antonio del Rio Chanona*

1:08 Paper 624c: A Surrogate-Based Framework for Feasibility Analysis and Optimization of Expensive Simulations — ***Huayu Tian**, Marianthi Ierapetritou*

1:27 Paper 624d: Data-Efficient Automated Tuning of Generic Control Structures Using Adversarially Robust Bayesian Optimization — ***Georgios Makrygiorgos**, Joel Paulson, Ali Mesbah*

1:46 Paper 624e: Accelerating Multiscale Global Optimization through Reduced Bayesian Optimization — ***Noah J. Wichrowski**, Georgios Psarellis, Anastasia Georgiou, Juan Bello-Rivas, Felix Dietrich, Jonathan Hauenstein, Ioannis G. Kevrekidis*

2:05 Paper 624f: Exploiting High-Throughput Experiments in Bayesian Optimization — ***Leonardo Gonzalez**, Victor Zavala*

2:24 Paper 624g: Snake: Bayesian Optimization Via Pathwise Exploration — ***Jose Pablo Folch**, Shiqiang Zhang, Robert M. Lee, Behrang Shafei, David Walz, Calvin Tsay, Mark van der Wilk, Ruth Misener*

2:43 Paper 624h: Optimization Under Uncertainty with Bayesian Hybrid Models — *Alexander Dowling, Kyla Jones, **Elvis Eugene**, Jialu Wang*

(625) Planning, Scheduling, Supply Chain and Logistics - I

Thursday, Nov 17, 12:30 PM
Phoenix Convention Center, W-101C

Styliani Avraamidou, Chair
Philip Tominac, Co-Chair

Sponsored by: Systems and Process Operations

12:30 Paper 625a: Optimal Scheduling with Preemptive Changeover Tasks: Solving a Benchmark Problem from the 80's — ***Pedro Castro***

12:48 Paper 625b: Distributional Reinforcement Learning for Chemical Production Scheduling and Supply Chain Optimization — ***Max Mowbray**, Antonio del Rio Chanona, Dongda Zhang*

1:06 Paper 625c: Workload Balancing in Periodic Distribution Scheduling and Routing Optimization — ***Aliakbar Izadkhah**, Akang Wang, José Miguel Laínez-Aguirre, Jose M. Pinto, Chrysanthos E. Gounaris*

1:24 Paper 625d: A Novel Framework for Supply Chain Optimization Under Major Disruptions — ***Oluwadare Badejo**, Marianthi Ierapetritou*

1:42 Paper 625e: Multiscale Integration for Sustainable and Resilient Distributed Energy Systems (DESs) — ***Natasha Chrisandina**, Shivam Vedant, Eleftherios Iakovou, Efstratios N. Pistikopoulos, Mahmoud El-Halwagi*

2:00 Paper 625f: New Product Introduction into a Pharmaceutical Manufacturing Network — ***Simon Brædder Lindahl**, Deenesh K. Babi, Gurkan Sin*

2:18 Paper 625g: Incentivizing Carbon Capture at Cellulosic Biorefineries: Integrated Optimization of Spatially Explicit Landscapes, Supply Chains, and Technology Portfolios — ***Eric O'Neill***, *Caleb Geissler, Christos Maravelias*

2:36 Paper 625h: Project Portfolio Optimization of Carbon Capture and Utilization Technologies for Oil and Gas Industries — ***Pooja Zen Santhamoorthy***, *Selen Cremaschi, Krishnaraj Sambath, Hariprasad J. Subramani*

(626) Effects of Confinement on Molecular Properties

Thursday, Nov 17, 12:30 PM
Phoenix Convention Center, N-222C

Liqun Zhang, Chair
Liangliang Huang, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

12:30 Paper 626a: Molecular Dynamics Simulations of Confined Deep Eutectic Solvents for Separations of Carbon Dioxide from Methane — ***Jiaming Xu***, *Francisco Hung*

12:45 Paper 626b: Dispersed State and Catalytic Activity of Nanoparticles Adsorbed in Mesoporous Silica — *Yingzhen Ma,* ***Bhuvnesh Bharti***

1:00 Paper 626c: Water in Zr-Based Metal-Organic Framework: Topology and Its Effect — ***Liangliang Huang***

1:15 Paper 626d: Molecular Dynamics Investigation on Branched Alkane-Air/Water Interfaces. — ***Praveen Pilyanam***, *Liqun Zhang*

1:30 Paper 626e: Tribology of Confined Imidazolium-Based ILs Using Atomistically-Detailed Molecular Simulations — *Daria Lazarenko,* ***Fardin Khabaz***

1:45 Paper 626f: Simulating Gas and Liquid Water in Faujasite — ***Richard Shiery***, *David Cantu*

2:00 Paper 626g: Interfacial Interactions between Confined Ionic Liquids and Mesoporous Silica — ***Andrew Drake***, *Folami Ladipo, Barbara Knutson, Stephen Rankin*

(627) Emulsions and Foams

Thursday, Nov 17, 12:30 PM
Phoenix Convention Center, N-232B

Esteban Urena-Benavides, Chair
Xiaoguang Wang, Co-Chair

Sponsored by: Interfacial Phenomena

12:30 Paper 627a: One-Pot CRISPR Reaction in Emulsions for High Throughput Screening of CRISPR-Cas9 Guide RNAs — ***Tinku Supakar***, *Eric Josephs*

12:45 Paper 627b: Stable Membraneless Complex Coacervate Microdroplet Emulsions — *Shang Gao, Advait Holkar,* ***Samanvaya Srivastava***

1:00 Paper 627c: Local Processes in Spontaneous Emulsification — ***Monicka Kullappan***, *Wesley D. Patel, Manoj K. Chaudhury*

1:15 Paper 627d: Continuous Emulsification in 3DP Fixed Beds: Drop Size Distribution and Emulsification Efficiency — ***Kaitlin Kay***, *Andres Hyer, Robert McMillin III, James K. Ferri*

1:30 Paper 627e: A Novel Hydrodynamic Film Drainage between an Emulsion Drop and a Surface to Predict Key Surface Wetting Rates — ***Sourojeet Chakraborty***, *Suraj Borkar, Arun Ramachandran*

1:45 Paper 627f: Comparison between Surfactants and Particles in Stabilizing Oil-in-Glycol Emulsions — ***Hari Katepalli***, *Daniel Dermody, Stephanie Hughes*

2:00 Paper 627g: Highly Stable Gas-in-Water Foams at High Salinity Stabilized with Nanoparticles and like-Charged Surfactants — ***Keith P. Johnston***, *Xiongyu Chen, Chang Da, Pinkeng Wu, Daniel Hatchell, Hugh Daigle*

2:15 Paper 627h: Capillary Foam Structure, Dynamics, and Flow Properties — ***J Carson Meredith***, *Sven H. Behrens, Omotola Okesanjo*

2:30 Paper 627i: Effect of Interfacial Properties on Foaming of per- and Polyfluoroalkyl Substances (PFAS) Solutions — ***Muchu Zhou***, *Stephen Kooker, Reza Foudazi*

2:45 Paper 627j: Growth and Coalescence of Nanoscopic Mesas in Stratifying Micellar Foam Films — ***Chenxian Xu***, *Yiran Zhang, Subinur I. Kemal, Vivek Sharma*

(628) Design and Analysis of Carbon Capture and Negative Emissions Technologies - Models

Thursday, Nov 17, 12:30 PM
Phoenix Convention Center, N-225B

Omar J. Guerra, Chair
Dora Lopez De Alonzo, Co-Chair
Shareq Mohd Nazir, Co-Chair

Sponsored by: Climate Change

12:30 Paper 628a: Techno-Environmental Analysis of Different Pre-Combustion Carbon Capture Technologies for Hydrogen Production from Waste — ***Alex Sebastiani***

12:48 Paper 628b: Incorporation of Market Signals for the Optimal Design and Operation of a Flexible Post-Combustion Capture System — ***Radhakrishna Tumbalam Gooty***, *Jaffer Ghouse, Quang Minh Le, Bhurisa Thitakamol, Sabereh Rezaei, Denis Obiang, Raghubir Gupta, S. James Zhou, Debangsu Bhattacharyya, David Miller*

1:06 Paper 628c: Optimisation of Carbon Capture and Storage Infrastructure in Wyoming to Reduce Carbon Emissions and Maximise Profits — ***Matthias Mersch***, *Niall Mac Dowell*

1:24 Paper 628d: Adsorption Kinetic Model for Direct Air Capture — ***James Akinjide***, *Aashish Priye, Joo-Youp Lee*

1:42 Paper 628e: Design of Passive Contactor Systems for Direct Air Capture — ***Xin Zhang***, *WonHee Lee, Sayan Banerjee, Christopher W. Jones, Ryan P. Lively, Matthew Realff*

2:00 Paper 628f: Process Analysis for Co-Removal of Methane and Carbon-Dioxide from Air — *Devesh Sathya Sri Sairam Sirigina, Aditya Goel,* ***Shareq Mohd Nazir***

2:18 Paper 628g: Feasibility of CO_2 Direct Air Capture Integration in Data Centers — ***Lindsey Hamblin***, *Matthew D. Green, Klaus S. Lackner*

2:36 Paper 628h: A Rooftop Approach for Direct Air Capture of Carbon-Dioxide — ***Shareq Mohd Nazir***, *Devesh Sathya Sri Sairam Sirigina, Mit Rakesh Surati, Shivani Ramprasad Jambur*

(629) Waste Plastic - Recycle, Reuse and Remediation Strategies

Thursday, Nov 17, 12:30 PM
Phoenix Convention Center, N-225A

Jeffrey Seay, Chair
Amy E. Landis, Co-Chair
Robert Peters, Co-Chair

Sponsored by: Solid and Hazardous Waste

12:30 Paper 629a: Utilization of Process Liquid from Hydrothermal Carbonization to Enhance Dehalogenation of Waste PVC — ***Vahab Ghalandari***, *Toufiq Reza*

12:48: Break

1:06 Paper 629c: Gasification of Waste Plastic to Enable a Circular Economy — ***Ping Wang***, *Nicholas C. Means, Fan Shi, Jonathan Lekse, McMahan L. Gray*

1:24 Paper 629d: A Generic Scenario Analysis of End-of-Life Plastic Management Concerning Chemical Additive Releases — ***John Chea***, *Austin Lehr, Kirti Yenkie, Joseph Stanzione III, Gerardo Ruiz-Mercado*

1:42 Paper 629e: The Removal of Nanoplastics from Water with Lignin-Based Hydrophobic Deep Eutectic Solvents As Novel Extractants — ***Yuxuan Zhang***, *Jameson Hunter, Usman Abbas, Qi Qiao, Qing Shao, Jian Shi*

2:00 Paper 629f: When and Where Do Bio-Plastics Make Sense? — ***Rachael Rothman***, *Maryam Hoseini, Stuart Walker, Tony Ryan*

2:18 Paper 629g: Many Happy Returns: Combining Environmental, Technological and Behavioural Sciences to Understand What Is Required to Make Reusable Packaging Sustainable. — ***Maryam Hoseini***, *Sarah Greenwood, Harriet Baird, Thomas Webb, Paul Mattinson, Patrick Fairclough, Rachael Rothman*

2:36 Paper 629h: Sustainable Use of Recycled Materials for the Cleaner Production of Value-Added Products — *Appala Naidu Uttaravalli, Hrithika Ganta, Meghana Bodhimisetty, Gopi Katiki, Likitha Gadde, Sanjana Mutyapu,* ***Bhanu Radhika Gidla***

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(630) Cell Culture Engineering and Biopharmaceutical Manufacturing

Thursday, Nov 17, 12:30 PM
Phoenix Convention Center, N-125B

Amir Sheikhi, Chair
Amol Janorkar, Co-Chair
Christopher Kieslich, Co-Chair

Sponsored by: Bioengineering

12:30 Paper 630a: Transferring CHO Cells from Monolayer to Suspension Culture By a New Design of Experiments - Superlative Box Design — ***Wanyue Cui***, *Shijie Liu*

12:48: Break

1:06 Paper 630c: Modeling and Detection of T Cell Exhaustion Markers in a Novel High-Density Centrifugal Bioreactor System with Application in Cancer Immunotherapy Treatments — ***Brenden Fraser-Hevlin***, *Kitana Kaiphanliam, Bernard Van Wie, William C. Davis*

1:24 Paper 630d: A Deep Examination of Carbon Feeding during the Production of Various Sized Vaccine and Therapeutic Candidates in *Komagataella Phaffi* — ***Joshua Hinckley***, *Carmen Elenberger, J. Christopher Love*

1:42 Paper 630e: Model-Based Insights on the Effect of Bioreactor pH and Temperature on N-Linked Glycosylation of Mabs Produced By CHO Cells — *Jayanth Venkatarama Reddy,* ***Katherine Raudenbush***, *Ou Yang, Aron Gyorgypal, Antash Chaturvedi, Shishir Chundawat, Marianthi Ierapetritou*

2:00 Paper 630f: Identification of Heritable Biomarkers That Characterize Resistance to Stress and Improved Productivity in CHO Cell Line Development — ***Spencer Grissom***, *Michael Saint-Antoine, Abhyudai Singh, Mark Blenner*

2:18 Paper 630g: Synthetic Gene Circuits for Therapeutic Platelet Production — ***Tara L. Deans***

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(631) Cells, Organs, and Labs on a Chip

Thursday, Nov 17, 12:30 PM
Phoenix Convention Center, N-126A

Adriana San Miguel, Chair
Quinton Smith, Co-Chair
Whitney Stoppel, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

12:30 Paper 631a: A Novel Microfluidic Device to Decipher the Interplay of Cellular Contractility and Electric Field during Galvanotaxis — ***Anindya Sen***, *Soontorn Tuntithavornwat, Bishwa Ranjan Si, Se Jong Lee, Kaustav Bera, Konstantinos Konstantopoulos*

12:48: Break

1:06 Paper 631c: Development of Heterogeneous Tumor Tissue-Mimicking Glioblastoma Organoids — *Seungjo (Joe) Park, Alexandra D. Avera,* ***Yonghyun (John) Kim***

1:24 Paper 631d: Comparison between Two Different 3D Printed Tumor-on-Chip Devices As Anti-Cancer Testing Platforms — ***Salvador Gallegos Martínez***, *Itzel Lara, David Choy Buentello, Grissel Trujillo de Santiago, Mario Moisés Álvarez*

1:42 Paper 631e: Islet-on-Chip Model for Type 2 Diabetes — ***Connor Wiegand***, *Ravi Krishnamurthy, Ipsita Banerjee*

2:00 Paper 631f: A Multi-Cellular Brain-on-Chip with Integrated Vasculature — ***Rebecca L. Pinals***, *Alice E. Stanton, Adele Bubnys, Dong Shin Park, Nhat Truong, Emre Abgas, Oyku Cerit, Benjamin James, Robert Langer, Li-Huei Tsai*

2:18 Paper 631g: Invited Speaker for Cells, Organs and Labs on a Chip — ***Whitney Stoppel***, *Quinton Smith*

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(632) General Topics in Synthetic Biology and Metabolic Engineering

Thursday, Nov 17, 12:30 PM
Phoenix Convention Center, N-125A

James Carothers, Co-Chair

Sponsored by: Bioengineering

12:30 Paper 632a: Expanding the Scope of Bacterial CRISPR Activation with PAM-Flexible dCas9 Variants — ***Ava Karanjia***, *Cholpisit Kiattisewee, Mateusz Legut, Samantha Koplik, Benjamin Kleinstiver, Neville Sanjana, James Carothers, Jesse Zalatan*

12:48 Paper 632b: Next Generation CRISPR-Cas Tools for Post-Transcriptional Gene Regulation in Bacteria — ***Ryan Cardiff***, *Cholpisit Kiattisewee, Jesse Zalatan, James Carothers*

1:06 Paper 632c: Development of a CRISPR Diversifying Base Editor in *Saccharomyces Cerevisiae* for Rapid Antibody Enhancement and Selection. — ***Andrew Cazier***, *John Blazeck*

1:24 Paper 632d: Establishment of an Efficient Bacterium-Yeast Consortium for Biosynthesis and Discovery of Strigolactones — ***Anqi Zhou***, *Sheng Wu, Kang Zhou, Yanran Li*

1:42 Paper 632e: Towards Programmable Interspecies Cell-Cell Communication in Bacterial Consortia: Synthetic Homoserine Lactone-Based Quorum Sensors for Gram-Positive *B. Subtilis* — ***Min Zeng***, *Biprodev Sarker, Lauren B. Andrews*

2:00 Paper 632f: Modular and Syntrophic Cocultures of *Clostridia* to Produce Isopropanol and C6-C8 Alcohols and Carboxylic Acids — ***Jonathan Otten***, *Hyeongmin Seo, Noah Willis, John Hill, Eleftherios Papoutsakis*

2:18 Paper 632g: Efficient Co-Utilization of Biomass-Derived Sugar Mixtures By Engineered *Escherichia coli* for Enhanced Production of Aromatic Biochemicals — ***Arren Liu***, *Michael Machas, Aditya Sarnaik, Arul Mozhy Varman, Xuan Wang, David Nielsen*

2:36 Paper 632h: Utilising a Genome Scale Metabolic Model to Design High-Producing CHO Cell Lines through Bi-Level Optimisation — ***Athanasios Antonakoudis***, *Alexandros Kiparissides, Cleo Kontoravdi*

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(633) Systems Biology for Engineering Metabolism

Thursday, Nov 17, 12:30 PM
Phoenix Convention Center, N-126B

Jason E. Shoemaker, Chair
Gregory Reeves, Co-Chair
Whitney Stoppel, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

12:30 Paper 633a: A Combined Analysis of Metabolic Networks and Transcriptomic Data to Predict the Impacts of Copper Deficiency on the Liver Metabolism — ***Naeun Lee***, *Joseph Brake, Heejeong Kim, Jaekwon Lee, Hyun-Seob Song*

12:48 Paper 633b: High-Performance Bioinformatics Workflow Incorporating Metabolomics Data Analysis, Processing, and Integration within the Exposome Concept. — ***Nafsika Papaioannou***, *Catherine Gabriel, Spyros Karakitsios, Dimosthenis Sarigiannis*

1:06 Paper 633c: A Computational Framework for Studying the Survival/Inhibition Mechanism of *Vibrio Cholera El Tor* with Evolving Metabolic Capability in a Glucose-Rich Environment — ***Faiz Khan Mohammad***, *Raghunathan Rengaswamy, Swagatika Sahoo*

1:24 Paper 633d: Developing a Machine Learning Model for Fitness Prediction in Multiplex Knockout *S. Cerevisiae* mutants — ***Michael Volk***, *Huimin Zhao*

1:42 Paper 633e: Tracking Pyrophosphate Metabolism and Evaluating Its Significance in the Bioprocessing of Lignocellulosic Biomass By *Clostridium Thermocellum* — ***Wheaton Schroeder***, *Tuen Kuil, Daniel Olson, Costas D. Maranas*

2:00 Paper 633f: Multi-Faceted Analysis Reveals the Metabolic Underpinnings of Overflow Metabolism in the Pathogenic *Staphylococcus Aureus* — *Adil Alsiyabi*, ***Rajib Saha***

2:18 Paper 633g: Invited Talk: Placeholder for Systems Biology for Engineering Metabolism Session — ***Whitney Stoppel***, *Jason E. Shoemaker, Gregory Reeves*

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(634) Chemical Modifications and Processing of Biomaterials I

Thursday, Nov 17, 12:30 PM
Phoenix Convention Center, N-228A

Zhaohui Tong, Chair

Sponsored by: Forest and Plant Bioproducts Division

12:30 Paper 634a: 4D Bio-Derived Photopolymers for 3D Printable Stimuli-Responsive Polymers — ***Andrew Weems***

1:00 Paper 634b: Simultaneous Heavy Metal Ion Capture and Detection Via Bio-Based Triboelectric Sensor — ***Geng-Sheng Lin***, *Haiyang Zou, Lan Gan, Zhaohui Tong, Yong Ding, Yongsheng Chen*

1:30 Paper 634c: Conversion of Lignocellulosic Biomass to Highly Functional Micro- and Nano-Materials for Water Treatment — ***Mica Pitcher***, *Amir Sheikhi, Breanna Huntington, Juliana Dominick*

2:00 Paper 634d: Tune Cellulose Nanocrystal Alignment By Combining the Additions of Electrolytes with Shear-Based Alignment — ***Ananya Ghosh***, *ZhongYang Cheng, Zhihua Jiang*

2:30 Paper 634e: Predicting the Morphological Properties of Activated Carbons Produced from Lignocellulosic Materials — ***Daniel Meadows***, *Delaney Clouse, Sushil Adhikari, Virginia Davis*

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(635) Developments in Alternative Fuels and Enabling Technologies

Thursday, Nov 17, 12:30 PM
Phoenix Convention Center, W-103A

Ashwin Ravichandran, Chair
Karthikeyan Ramasamy, Co-Chair

Sponsored by: Fuels and Petrochemicals Division

12:30 Paper 635a: First European Demonstration Plant for the Synthesis of Renewable Ome Fuels — ***Alvaro Ferre***, *Johannes Voggenreiter, Christian F. Breitkreuz, Denis Worch, Udo Lubenau, Hans Hasse, Jakob Burger*

12:47 Paper 635b: Additive Solutions for Renewable Fuels and Feedstocks — ***Daniel Dreyer***, *Nestor Soriano Jr., Ashish Dhawan, Oussama Zenasni, Josep Marca, Elizabeth Balapitiya*

1:04 Paper 635c: CFD Modeling Development of Onboard Absorptive Hydrogen Storage on Coal-Derived Activated Carbon for Light-Duty Vehicles — ***Subhodeep Banerjee***, *Ki-Joong Kim, Christopher Matranga, Mehrdad Shahnam, William Rogers*

1:21 Paper 635d: Durability of Wellbore Cements Under Cyclic Loading Temperatures: Impacts of Graphene Nanoplatelets (GNPs) Enhanced Cements and Fracturing Fluids Contamination — ***Havila Jupudi***, ***Gabriel Awejori***, *Cody Massion, Mileva Radonjic*

1:38 Paper 635e: Modelling and Experiments on the Impact of Mild and Biodegradable Surfactants on Hythane Gas Hydrate Formation — ***Bhavikkumar Mahant***, *Omkar Singh Kushwaha, Rajnish Kumar*

1:55 Paper 635f: Investigating the Performance of the Pyrolysis Process for Different Feedstocks — ***Hasan Al-Abedi***, ***Haider Al-Rubaye***, *Joseph Smith*

2:12 Paper 635g: Total Acid Number Reduction of Renewable Thermal Deoxygenation (TDO) Oil for Coprocessing in Refineries — ***Sampath Karunarathne***, *Matthew J. Kline, M. Clayton Wheeler*

2:29 Paper 635h: Investigation of Thermos-Kinetic Study of Waste Motor Oil Pyrolysis Utilizing the Thermogravimetric Analysis and Self-Designed Batch Scale Pyrolyzer — ***Asmita Mishra***, *Bhim Charan Meikap*

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(636) Biopolymers

Thursday, Nov 17, 12:30 PM
Phoenix Convention Center, N-122B

Yeongseon Jang, Chair
Monirosadat Sadati, Co-Chair

Sponsored by: Polymers

12:30 Paper 636a: Photoactive C-Phycocyanin Assemblies: From Food Colorants to Tunable Biofunctional Materials — *Ying Li, Richard Gillilan*, ***Alireza Abbaspourrad***

1:00 Paper 636b: High-Throughput Tool Development for Protein Materials Expression and Screening — ***Melody Morris***, *Yun Jung Yang, Bradley Olsen*

1:15 Paper 636c: A Study of Recombinant Fusion Proteins Self-Assembly in Macromolecularly Crowded Conditions — ***Jooyong Shin***, *Yeongseon Jang*

1:30 Paper 636d: Self-Assembly of Biosynthetic Protein Polyelectrolytes and Block Copolymers — *Justin Horn, Yuncan Zhu, So Yeon Ahn*, ***Allie Obermeyer***

1:45 Paper 636e: Surface Modification of Polymer Nanoparticles for Drug Delivery and Their Behavior in Blood Plasma Using Nanoparticle Tracking Analysis — *Aida López Ruiz, Mark Bannon*, ***Kathleen McEnnis***

2:00 Paper 636f: Controlling Moisture Sensitivity in Cellulose-Based Films — ***Tanner Hickman***, *Natalie Stingelin, J Carson Meredith*

2:15 Paper 636g: In-Vitro Adsorption of Paracetamol Overdose Using Olive Leaves Biomass — *Saif Al Janabi, Basel Al-Saida, Arwa Sandouqa*, ***Reyad Shawabkeh***

2:30 Paper 636h: Synthesizing Thermosetting Polymers from Birch Bark Extract — ***John Chea***, *Kylie Howard, David Fenton, Heather LaFrance, James Newell, Kirti Yenkie, Joseph Stanzione III*

2:45 Paper 636i: Spin Coating Photosystem I-PEDOT:PSS Composite Films — ***Marc Nabhan***, *G. Kane Jennings, David Cliffel, Carlos Silvera Batista*

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(637) Hydrogel Biomaterials II: Cell Instructive Platforms

Thursday, Nov 17, 12:30 PM
Phoenix Convention Center, N-121B

Amir Sheikhi, Chair
Marjan Rafat, Co-Chair
Mai Ngo, Co-Chair
Mark Tibbitt, Co-Chair

Sponsored by: Biomaterials

12:30 Paper 637a: Engineering Supramolecular Shear-Thinning Hydrogels to Promote Oligodendrocyte Progenitor Cell Transplantation for Demyelinating Diseases — ***Ashis Kumar Podder***, *Mohamed Mohamed, Georgios Tseropoulos, Richard Seidman, Jessie Polanco, Fraser Sim, Stelios Andreadis*

12:45 Paper 637b: Engineered Matrices Reveal Stiffness-Mediated Progression of Fatty Liver Disease — ***Aidan Gilchrist***, *Yueming Liu, Yuan Guan, Sarah C. Heilshorn, Gary Peltz*

1:00 Paper 637c: Development and Characterization of Injectable, Guest-Host Hydrogels for Neural Tissue Engineering Applications — ***Gregory Jensen***, *Sarah Stabenfeldt, Julianne Holloway*

1:15 Paper 637d: Mechanical Characterization of Elastic and Viscoelastic Polyacrylamide Hydrogels for Cell-Substrate Interaction Studies — ***Ariell Smith***, *Roberto Andresen Eguiluz, Arvind Gopinath*

1:30 Paper 637e: Characterization of Length-Scale Dependent Rheology Using Bi-Disperse Multiple Particle Tracking during Cell-Material Interactions — *John A. McGlynn, **Kelly M. Schultz***

1:45 Paper 637f: Multifunctional Materials for the Adsorption of Metabolic Toxins with a Focus on Chronic Kidney Disease — ***Matthew Garnett**, Symone Alexander*

2:00 Paper 637g: Design, Synthesis, Characterization, and Evaluation of Synthetic Scaffolds for 3D T Cells Culture and Co-Cultures — ***Gaby Lizana-Vasquez**, Madeline Torres Lugo*

2:15 Paper 637h: A Biomimetic Hyaluronic Acid Hydrogel Models Mass Dormancy in Brain Metastatic Breast Cancer Spheroids — ***Raghu Vamsi Kondapaneni**, Lalita A. Shevde, Shreyas Rao*

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(638) Polymer Thin Films, Confinement, and Interfaces I

Thursday, Nov 17, 12:30 PM
Phoenix Convention Center, N-122A

Kathleen McEnnis, Chair
Julie Albert, Co-Chair
Jean-Francois Louf, Co-Chair
Rong Yang, Co-Chair

Sponsored by: Polymers

12:30 Paper 638a: Membrane Selective Layers Formed from Amphiphilic Polyampholytes and Amphiphilic Polyelectrolyte Bilayers — ***Ayse Asatekin***

1:00 Paper 638b: Altering the Interfacial Chemical Makeup to Manipulate the Distribution of Ion Conduction Environment across Ionomeric Materials — ***Shudipto Dishari***

1:15 Paper 638c: Sequence-Defined Polymer Brushes for Surface Nanopatterning Towards Directed Biomolecular Assemblies — ***Beihang Yu**, Boyce Chang, Whitney Loo, Scott Dhuey, Paul D. Ashby, Michael Connolly, Kathleen Ryan, Grigory Tikhomirov, Ronald N. Zuckermann, Ricardo Ruiz*

1:30 Paper 638d: Engineering of Super-Hydrophilic Coatings through Surface-Initiated Polymerization — *Michele Fromel, **Christian Pester***

1:45 Paper 638e: Engineering "Solvation" in All-Dry Polymerization — ***Pengyu Chen**, Deborah Zhang, Jingjie Yeo, Rong Yang*

2:00 Paper 638f: Chemical Vapor Deposition of Dicyanate Ester Polymer Films — ***Shayna Rumrill**, Kenneth Lau*

2:15 Paper 167k: Can Short Linear Block Copolymers Stabilize Perpendicular Lamellae in Linear-Cyclic Block Copolymer Blend Films? — ***Rahul Kumar**, Wenqi Yang, Julie Albert, Henry Ashbaugh*

2:30 Paper 638h: Kinetically-Limited Deposition of Polymer Films By Initiated Chemical Vapor Deposition — ***Varun Prasath**, Kenneth Lau*

2:45 Paper 638i: Nanoconfined Benzyl Methacrylate Radical Polymerization — *Chunhao Zhai, Bryan Vogt, **Sindee Simon***

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(639) Polymer Viscoelasticity: Mechanics, Processing, and Rheology II

Thursday, Nov 17, 12:30 PM
Phoenix Convention Center, N-121C

Gregory McKenna, Chair
Nader Taheri-Qazvini, Co-Chair
Amanda Marciel, Co-Chair
Sara Hashmi, Co-Chair

Sponsored by: Polymers

12:30 Paper 639a: Recyclable Dynamic Covalent Polymer Networks: Roles of Viscoelasticity and Rheology in Reprocessing and Robust Sustainable Response — ***John Torkelson***

1:00 Paper 639b: Flow-Induced Configuration Microphase Separation and Crystallization of Entangled Polyethylene Under Uniaxial Extensional Flows — ***Mohammad Hadi Nafar Sefiddashti**, Brian J Edwards, Bamin Khomami*

1:15 Paper 639c: Predicting the Plateau Modulus from Molecular Parameters of Conjugated Polymers — *Abigail Fenton, **Renxuan Xie**, Chad R. Snyder, Enrique D. Gomez, Ralph H. Colby*

1:30 Paper 639d: Characterization of the Network Structure of Ancient Ambers — *Dejie Kong, Yan Meng, **Gregory McKenna***

1:45 Paper 639e: Entanglement Kinetics in the Discrete Slip-Link Model — ***Benjamin Dolata**, Jonathan Seppala*

2:00 Paper 639f: Effect of Concentration of Hydrophobic Components and Environmental Conditions on the Mechanical Properties of a Stretchable Hydrogel — *Anandavalli Varadarajan, **Santanu Kundu***

2:15 Paper 639g: Thermal Properties and Crystallinity of Poly (ε-caprolactone) (PCL) and MgO Incorporated PCL Nanofibers — ***Nabila Shamim**, Daisaku Gicheha*

2:30 Paper 604h: Centrifugal Force Spinning and Volatile-Entangled Vs Extensibility-Enriched Spinnability of Polymer Solutions — ***Cheryl Slykas**, Carina Martinez, Louie Edano, Vihar Trada, Jorge Merchiers, Naveen Reddy, Vivek Sharma*

2:45 Paper 639i: Rheology of Ring Polymers — *Dongjie Chen, Julia A. Kornfield, Judit E. Puskas, Kristof Molnar, Carin A. Helfer, Hojin Kim, Gabor Kaszas, **Gregory McKenna***

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(640) Advances in Drug Discovery Processes (including HTE): Protein Engineering Approaches with Target Therapeutic Applications

Thursday, Nov 17, 12:30 PM
Phoenix Convention Center, N-123

Huiquan Wu, Chair
Curtis Martin, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

12:30 Paper 640a: Intelligent High-Throughput Intervention Testing Platform in *Daphnia* — ***Yongmin Cho**, Marc Kirschner, Leonid Peshkin*

12:51 Paper 640b: Cellular Proton Motive Force: A Therapeutic Target for Eradicating Methicillin-Resistant *Staphylococcus Aureus* Persister Cells — ***Sreyashi Ghosh**, Sayed Golam Mohiuddin, Pouria Kavousi, Mehmet Orman*

1:12 Paper 640c: Identification of Apolipoprotein E4 Inhibitors for Alzheimer's Disease Therapy through Large-Scale Virtual Screening — ***Zuyi Huang**, Emily Krass, **Tianhua Zhai***

1:33 Paper 640d: Polymer Lung Surfactant: A First-in-Class Synthetic Surfactant Therapeutic for Acute Respiratory Distress Syndrome (ARDS) — ***You-Yeon Won**, Daniel Fesenmeier, Seyoung Kim*

1:54 Paper 640e: An Innovative Therapeutic Fusion Protein Approach for Chronic Wound Healing — ***Hazim Aljewari**, Shadrach Ibinola, Stephanie Beitle, Ahmed Elmasheiti, Josh Sakon, Robert Beitle*

2:15 Paper 640f: Peg-Conjugated Extracellular Mega-Hemoglobin for Diverse Oxygen Therapeutic Applications — ***Chintan Savla***

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(641) Computational solid state pharmaceutics II

Thursday, Nov 17, 12:30 PM
Phoenix Convention Center, N-122C

Yuriy Abramov, Chair
Ebenezer Ojo, Co-Chair
Daniel Hallow, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

12:30 Paper 641a: Comparison of One Dimensional and Two-Dimensional Population Balance Model for Optimization of a Crystallization Process — ***Bhavik Mehta, PhD**, Niall Mitchell, Cameron Brown, Sebastion Davidson, Alastair J. Florence*

12:51 Paper 641b: In-Depth Analysis of the Impacts of Material Properties on Size Distributions in Continuous Twin-Screw Wet Granulation to Construct a Generic 1D Population Balance Model — ***Kensaku Matsunami**, Ana Alejandra Barrera Jimenez, Michiel Peeters, Daan Van Hauwermeiren, Thomas De Beer, Ingmar Nopens*

1:12 Paper 641c: Use of gPROMS for Film Coating Processes - Streamlined QbD Process Development — ***James Miesle***, *Salvador Garcia Munoz*

1:33 Paper 641d: Towards Optimized Pharmaceutical Freeze-Drying Processes Via Controlled Nucleation: Mechanistic Modeling of Vacuum-Induced Surface Freezing — ***Leif-Thore Deck***, *Andraž Košir, Marco Mazzotti*

1:54 Paper 641e: Modelling the Stress Distribution in Tablet Coatings Exposed to Rapid Environmental Changes — *Venugopala S. Punati,* ***Mahesh S. Tirumkudulu***, *Ashwinkumar Jain, Daniel O. Blackwood, Alfred Berchielli, Pankaj Doshi*

2:15 Paper 641f: Modeling the Steady State of a Spray Drying Unit with Drying Gas Recirculation Accounting for Complex Thermodynamics Using Sequential Simulation — ***Salvador Garcia Munoz***

2:36 Paper 641g: A Novel Adaptive Residence Time Distribution (RTD) Modelling Toolbox — ***Ravendra Singh***, *Fernando Muzzio*

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(642) Highly Selective Separations with Membranes

Thursday, Nov 17, 12:30 PM
Phoenix Convention Center, N-221C

Siamak Nejati, Chair
Manish Kumar, Co-Chair
Ngoc Bui, Co-Chair

Sponsored by: Membrane-Based Separations

12:30 Paper 642a: Thermodynamic Gate-Opening Behavior Study on Network Nanostructured ZIF-8 to Control Gas Transport Selectivity — ***Hyunhee Lee***, *Zachary Smith*

12:51 Paper 642b: The Mechanism of Light Gas Transport through Configurational Free Volume in Glassy Polymers — ***William Box***, *Zihan Huang, Ruilan Guo, Michele Galizia*

1:12 Paper 642c: Selective H_2S/CO_2 Separation Using Sterically Hindered Amine Membranes — ***Shraavya Rao***, *Xuepeng Deng, Yang Han, Li-Chiang Lin, W.S. Winston Ho*

1:33 Paper 642d: Microstructural Modification of Polycrystalline ZIF-8 Membranes By an Additive for Enhanced Propylene/Propane Separation Performance — ***Donga Kang***, *Hae-Kwon Jeong*

1:54 Paper 642e: Separation of HFC-32 and HFC-125 Using Amorphous Copolymers of Perfluoro(butenyl vinyl ether) (PBVE) and Perfluoro(2,2-dimethyl-1,3-dioxole) (PDD) — ***Abby Harders***, *Luke Wallisch, Mark Shiflett, Erin Sturd*

2:15 Paper 642f: Shape-Selective Filtration of Nanomaterials and Proteins Using Lamellar Block Copolymer-Based Slit Membranes — ***Maninderjeet Singh***, *Alamgir Karim*

2:36 Paper 642g: Conjugated Polymers for Molecular Separation — ***Christopher Merkel***, *Febby Andini, Syed Ibrahim Gnani Peer Mohamed, Mona Bavarian, Siamak Nejati*

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(643) Innovation in Membrane Manufacturing

Thursday, Nov 17, 12:30 PM
Phoenix Convention Center, N-131B

Jeffrey McCutcheon, Chair
Mayur Ostwal, Co-Chair

Sponsored by: Membrane-Based Separations

12:30 Paper 643a: Novel Electrospun Membrane Structures for Reverse Osmosis, CO_2 Stripping and Membrane Distillation — ***Sandra Kentish***, *Daniel Heath, Seungju Kim*

12:51 Paper 643b: Optimizing Fabrication of Polysulfone Ultrafiltration Membranes Using a Green Solvent, Cyrene — ***Cannon Hackett***, *David Hale, Ranil Wickramasinghe, Xianghong Qian, Audie Thompson*

1:12 Paper 643c: 3D Printing of Thin Film Composite Membranes for Nanofiltration and Beyond — ***Jeffrey McCutcheon***, *Xin Qian, Mayur Ostwal, Edward Wazer*

1:33 Paper 643d: Innovative Manufacturing of Porous Oxide Hollow Fiber Membranes — ***Chen Zhang***

1:54 Paper 643e: An Innovative One-Step Approach to Fabricate MOF-Containing Asymmetric Mixed-Matrix Membranes for Gas Separation — ***Yinying Hua***, *Sunghwan Park, Hae-Kwon Jeong*

2:15 Paper 643f: Prospect of Using Machine Learning for Evaluating Gas Separation Membranes' Transport Properties and Assisted Fabrication — ***Arash Tayyebi***, *Ali Alshami*

2:36 Paper 643g: Intrinsically Porous, Chemically Tunable, and Mixed Matrix 3D Printed Membranes for Targeted Purification — ***Ryan Mulvenna***, *Michael Scalzo, Abdollah Khosravanian, Huacheng Zhang, Benny D. Freeman, Timothy F. Scott, Matthew R. Hill*

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(644) Membrane-Based Organic Solvent Separations

Thursday, Nov 17, 12:30 PM
Phoenix Convention Center, N-132A

Ryan P. Lively, Chair
Neel Rangnekar, Co-Chair

Sponsored by: Membrane-Based Separations

12:30 Paper 644a: Thin-Film Covalent Organic Framework Membranes Made By Interfacial Synthesis for Organic Solvent Nanofiltration — ***Xiaoli Ma***, *Zhiqin Qiang, Rahul Sampat Khandge*

12:51 Paper 644b: Quantifying Self-Diffusion of Mixed and Pure Organic Liquids in ZIF-Based Mixed Matrix Membranes By NMR — *Amineh Baniani, Matthew Rivera, Ryan P. Lively,* ***Sergey Vasenkov***

1:12 Paper 644c: Tuning Polyimide Thin Film Composite Membranes for Organic Solvent Reverse Osmosis Separations Via Boc Protected Amine Solid-State Crosslinking — ***Yacine Feliachi***, *Ryan P. Lively, M.G. Finn*

1:33 Paper 644d: Mass Transport Modeling in Membrane-Based Chemical Separations — ***Akshay Deshmukh***, *Mathew M. Swisher, Nicolas G. Hadjiconstantinou, John H. Lienhard*

1:54 Paper 644e: Tunable Bottlebrush Membranes for Organic Solvent Nanofiltration — ***Pranav Ramesh***, *Mirco Sorci, Bratin Sengupta, Miao Yu, James (Chip) Kilduff, Georges Belfort*

2:15 Paper 644f: Highly Interconnected Pores in Hybrid Nanofilms for Ultrafast Solvent Transport with Precise Molecular Separation — ***Bratin Sengupta***, *Qiaobei Dong, Dinesh Behera, Fanglei Zhou, Ji Jiang, Georges Belfort, Miao Yu*

2:36 Paper 644g: Structure Design of Nanoporous Multilayer Graphene Membrane for Organic Solvent Nanofiltration — ***Dae Woo Kim***

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(645) Molecular Simulations for Designing Adsorbents and Adsorption Processes

Thursday, Nov 17, 12:30 PM
Phoenix Convention Center, N-130

Alexander Neimark, Chair
Peter Ravikovitch, Co-Chair

Sponsored by: Adsorption and Ion Exchange

12:30 Paper 645a: Effect of Energetical and Geometrical Heterogeneity of Kerogen on BET Surface Area Characterization and Methane Adsorption — *Yingnan Wang, Wanying Pang,* ***Zhehui Jin***

12:45 Paper 645b: Deformation of Nanoporous Carbons Induced By Multicomponent Adsorption: Insight from the SAFT-DFT Model — ***Nicholas Corrente***, *Alexander Neimark*

1:00 Paper 645j: Designing Highly-Selective Sorbents for Diagnosing Respiratory Disease Via Breath Analysis — ***Scott Bobbitt***, *Michael E. Chandross, Jason Sammon, Jacob I. Deneff, Dorina F. Sava Gallis*

1:15 Paper 645d: Flat-Histogram Simulations of Water in MOFs: Advanced Strategies for Overcoming Sampling Challenges — ***Daniel Siderius***, *Harold Hatch, Vincent K. Shen*

1:30 Paper 572f: An Efficient Featurization Scheme for Machine-Learning Predictions of Diverse Molecules in Metal-Organic Frameworks — ***Sihoon Choi***, *Xiaohan Yu, David Sholl, Andrew Medford*

1:45 Paper 645f: Impact of Metal-Organic Framework Characteristics on Electrostatic Interactions for Gcmc-Simulated Adsorption — ***Brandon Bout***, *Krista Walton*

2:00 Paper 645g: In silico Screening of Metal-Organic Frameworks for Harvesting Atmospheric Water — ***Li-Chiang Lin***, *Archit Datar, Yi-Ming Wang, Zhi-Xun Xu, Matthew Witman*

2:15 Paper 645h: Modelling Hierarchical Carbon-Based Materials for CO_2 Capture and Separation — ***Daniel Bahamon***, *Nour Alkhatib, Mohammad Abu Zahra, Maryam Khaleel,* ***Lourdes Vega***

2:30 Paper 645i: Modeling of Adsorption and Diffusion of Chemical Agents and Simulants in UiO-66 — ***Chinmay Mhatre***, *Jacob Wardzala, Meiirbek Islamov, Paul Boone, Christopher E. Wilmer, Karl Johnson*

2:45: Break

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(646) Particle Formation and Crystallization Processes from Liquids, Slurries, and Emulsions

Thursday, Nov 17, 12:30 PM
Phoenix Convention Center, N-131A

Manish Kelkar, Chair
Daniel J. Jarmer, Co-Chair

Sponsored by: Crystallization and Evaporation

12:30: Introductory Remarks

12:33 Paper 646b: Crystallization Kinetics and Solubility of Amoxicillin Trihydrate in the Presence of Synthesis Substrates — ***Patrick Harris***, *Hossein Salami, Ronald Rousseau, Martha Grover, Andreas Bommarius*

1:02 Paper 646c: Application of Silane-Modified Silica of Different Morphologies Towards the Demulsification of Water in Oil Emulsions — ***Anirban Ghosh***, *Michael Miranda, Clint Aichele*

1:31 Paper 646d: Segmented Flow Crystallization of Paracetamol Via Microdroplet Cooling — ***Jacob Crislip***, *Januario da Costa, Andrew R Teixeira*

2:00 Paper 646e: Impurity Inclusion and Crystallization Performance in Batch and Continuous Mode — *Christine Darmali,* ***Nima Yazdanpanah***, *Shahnaz Mansouri, Zoltan Nagy, Meng Wai Woo*

2:29: Concluding Remarks

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(647) PSA/TSA and Adsorption Processes Design and Scale-up

Thursday, Nov 17, 12:30 PM
Phoenix Convention Center, N-131C

Reza Haghpanah, Chair
Julien Cousin-Saint-Remi, Co-Chair

Sponsored by: Adsorption and Ion Exchange

12:30 Paper 647a: Practically Achievable Process Limits for a Temperature Swing Adsorption Process for CO_2 Capture from Ngcc Flue Gas — ***Yogashree Bharath***, *Kasturi Nagesh Pai, Phuc-Tien Thierry, Samuel Lethier, Philip Llewellyn, Cecile Pereira, Veronique Pugnet, Arvind Rajendran*

12:46 Paper 647b: Temperature-Vacuum Swing Adsorption Process for Direct Air Capture of CO_2 — ***James A. Ritter***, *Marjorie A. Nicholson, Armin Ebner*

1:02 Paper 647c: Efficient Surrogate Optimization of Pressure-Vacuum Swing Adsorption Processes for Post-Combustion CO_2 Capture — ***Adam Ward***, *Ronny Pini*

1:18 Paper 647d: On the Use of Absolute and Excess Isotherms in Adsorption Processes: H_2 PSA As a Case Study. — ***Riccardo Rea***, *Mauro Luberti, Stefano Brandani, Enzo Mangano*

1:34 Paper 647e: Blue H_2 Production of 12-Bed PSA Process Integrated with CO_2 Absorption Process from Smr Syngas — ***Jun-Ho Kang***, *Hyun-Taek Oh, Hyeon-Hui Lee, Chang-Ha Lee*

1:50 Paper 647f: Evaluation of Adsorbent Performance By Optimal Temperature Swing Adsorption Process — ***Yuchi Sugiura***, *Tomoyuki Yajima, Yoshiaki Kawajiri*

2:06 Paper 647g: Superstructure Optimization of Pressure Vacuum Swing Adsorption Processes — ***Kasturi Nagesh Pai***, *Reza Haghpanah, William Edsall*

2:22: Break

2:38 Paper 647i: A Strategy for Optimal Process Design and Operation of a Pressure Swing Adsorption (PSA) System through Pressure Equalisation and Co-Current Depressurisation — *Yan Chen,* ***Hyungwoong Ahn***

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(648) Climate Change and Engineering Sustainability

Thursday, Nov 17, 12:30 PM
Phoenix Convention Center, N-226A

Raymond Smith, Chair
Simona Liguori, Co-Chair

Sponsored by: Sustainability Science and Engineering

12:30 Paper 648a: Modeling Direct and Indirect Carbon Flows in the Chemicals and Materials Industry to Enable a Net-Zero Emissions Future — ***Amrita Sen***, *George Stephanopoulos, Bhavik Bakshi*

12:53 Paper 648b: Comparison of Decarbonization Effectiveness Among Steelmaking, Cement, and Aluminum at the Country Level — ***Lingyan Deng***, *Sydney Johnson, Emre Gençer*

1:16 Paper 648c: Biofilm-Based Cultivation of Methanotroph-Photoautotroph Coculture – a Highly Effective Biogas Valorization Technology — *Kiumars Badr, Q. Peter He,* ***Jin Wang***

1:39 Paper 648d: Efforts to Reduce GHG Emission Footprint of Magnesium Industries By Deep Eutectic Solvents — ***Thomas Quaid***, *Toufiq Reza*

2:02 Paper 648e: Rational Design of Low Global Warming Potential Drop-in Replacements through a 3E (Energy, Environmental and Economics) Analysis — ***Carlos Albà Garriga***, *Ismail Alkhatib, Felix Llovell, Lourdes Vega*

2:25 Paper 648f: Green H2 Fuel for Industry and Maritime Sector Decarbonization: Impacts on Hydrogen Economy for Qatar — *Kazi Khoda,* ***Fadwa Eljack***

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(649) CO_2 Capture for Power Generation

Thursday, Nov 17, 12:30 PM
Phoenix Convention Center, N-226C

David Hopkinson, Chair
Zachary Smith, Co-Chair

Sponsored by: Sustainable Energy

12:30 Paper 649a: CO_2-Binding Organic Liquids (CO_2BOLs) Enabling Energy- and Cost-Effective Carbon Capture from Point-Sources — ***Yuan Jiang***, *Paul Mathias, Charles J. Freeman, Richard Zheng, David J. Heldebrant*

12:45 Paper 649b: Introducing Solid with Infused Reactive Liquid (SWIRL) for Effective CO_2 Capture — ***Mohsen Yeganeh***, *Arben Jusufi, Shane Deighton, Matthew S. Ide, Michael Siskin, Aditya Jaishankar, Pedro Bertolini, Charles Maldarelli, Bharath Natarajan, Jessica Vreeland, Mark King, Andrew Konicek*

1:00 Paper 649c: Investigation of Preferential CO_2 Binding on Lignin-Derived Carbon Quantum Dots through Molecular Dynamics Simulations — ***Michael Broud***, *Lu Yu, David P. Harper, David Keffer*

1:15 Paper 649d: Isotherm Modeling and Techno-Economic Optimization of Contactor Technologies for a New Tetraamine-Appended MOF for CO2 Capture from Ngcc Plants — ***Ryan Hughes***, *Daison Manuel Yancy Caballero, Miguel A. Zamarripa, Benjamin P. Omell, Michael S. Matuszewski, Debangsu Bhattacharyya*

1:30 Paper 649e: Electrified Low-Temperature Process for CO_2 Capture and Conversion — ***Kangze Shen**, Carlos Morales-Guio*

1:45 Paper 649f: Utilizing Direct Air Capture for Reduced Power Plant Fuel Consumption and Lower Cost Agriculture Production/ Bio-Sequestration — ***Brian Kolodji**, Marc Straub, Bruce Kimball, Brian Marsh, Paramjit Dosanjh, Manuel Aguayo*

2:00 Paper 649g: Multi-Concentration CO_2 Capture at a 0.7 MWe Post-Combustion Pilot Plant — ***Reynolds Frimpong**, Heather Nikolic, Kunlei Liu*

2:15 Paper 649h: Biomass Cofiring with Postcombustion Carbon Capture Baseline Testing at Und Eerc — *John Kay, **Joshua Stanislowski***

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(650) Life Cycle Analysis of Bio-Based Fuels, Energy, and Chemicals

Thursday, Nov 17, 12:30 PM
Phoenix Convention Center, N-226B

Yuan Yao, Chair
David Shonnard, Co-Chair

Sponsored by: Sustainable Biorefineries

12:30 Paper 650a: Life Cycle Assessment of Jet Fuel Produced from IH2-Cool Gtl Integrated Process — *Robert Handler, **David Shonnard**, Terry Marker*

12:55 Paper 650b: Evaluating the Environmental Impact of Circular Economy Strategies in Biobased Industries Using a Hybrid Input-Output Model Built on Process-Driven Physical Data — ***Miriam Stevens**, Shweta Singh*

1:20 Paper 650c: Life Cycle Assessment of a Flow Synthesis of Paracetamol from Bio-Waste Feedstock β-Pinene — ***Sabine Hallamasek**, Vera Ubbenjans, Alexei A. Lapkin*

1:45 Paper 650d: Multi-Scale Life Cycle Environmental Impacts of Urban Waste Valorization — *Kai Lan, Bingquan Zhang, **Yuan Yao***

2:10 Paper 650e: Economic and Environmental Impact of Bioplastics Manufacturing Expansion in the US Using Environmentally Extended Input-Output Analysis — ***Apoorva Bademi**, Shweta Singh*

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(651) CO2 Upgrading II: From Fundamental to Applied CO2 Electrocatalysis I

Thursday, Nov 17, 3:30 PM
Phoenix Convention Center, N-128A

Mohammad Asadi, Chair
Nitish Mittal, Co-Chair

Sponsored by: Catalysis

3:30 Paper 651a: Electrochemical CO_2 Reduction: From Fundamentals to More Applied Systems — ***Thomas Jaramillo***

4:10 Paper 651b: Highly Efficient C_{2+} Alcohols Electrosynthesis Enabled By Bi-Metal Cu-Based Alloys — ***Mohammadreza Esmaeilirad**, Ahmad Mosen Harzandi, Mohammad Asadi*

4:28 Paper 651c: Decoupling of Intrinsic Kinetics of Electrochemical CO_2 Reduction on Flat and Porous Copper Via Dimensionless Characterization of External and Internal Mass Transfer — ***Joonbaek Jang**, Maximilian Winzely, Martina Rüscher, Dolores Rodriguez, Carlos Morales-Guio*

4:46 Paper 651d: Determining Effects of Interfacial Potential, pH and High Coverages on in-Situ Structure and Kinetics for CO_2 Reduction on Cu(100) — ***Ankita Morankar**, Siddharth Deshpande, Jeffrey Greeley*

5:04 Paper 651e: Benchmarking Solvation Effects for Electroreduction of CO over Cu-Based Catalysts — ***Viswanath Pasumarthi**, Stephen E. Weitzner, Sneha Akhade, Joel B. Varley, Frank Abild-Pedersen, Michal Bajdich*

5:22: Break

5:40 Paper 651g: Recovering Carbon Losses in CO_2 Electrolysis Using a Solid Electrolyte Reactor — ***Haotian Wang***

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(652) Homogeneous Catalysis

Thursday, Nov 17, 3:30 PM
Phoenix Convention Center, N-127B

Deven Swapneshu Baser, Chair
Nicholas Brunelli, Co-Chair

Sponsored by: Catalysis

3:30 Paper 652a: Investigating Reaction Mechanisms Using Synthetic and Spectroscopic Tools — ***Nicholas Brunelli**, Nitish Deshpande, Montgomery Gray, Michael Hines, T.V. Rajanbabu*

3:50 Paper 652b: A Localized Enantioselective Catalytic Site on Short DNA Sequences and Their Amphiphiles — ***Danyu Wang**, Jun Guo, Evangelia Pantatosaki, Huihui Kuang, George K. Papadopoulos, Michael Tsapatsis, Efrosini Kokkoli*

4:10 Paper 652c: Quick and Accurate Estimates of Mutation Effects on Relative Activity of Enzymes from Molecular Simulations with Restrained Transition States — ***Tucker Burgin**, David Beck, Jim Pfaendtner*

4:30 Paper 652d: Sequential Oxidation of Glucose Using Glucose Oxidase and Au and Aupd Nanoparticles — *Joseph Brindle, Rashmi Charde, **Michael Nigra***

4:50 Paper 652f: Enantioselective Catalysts Based on Metal-Organic Framework Supported Nucleotides — ***Danyu Wang**, Zhe Li, Tianyi Luo, Michael Schmithorst, Sunghwan Park, Wenqian Xu, Brandon Bukowski, Bradley F. Chmelka, Efrosini Kokkoli, Michael Tsapatsis*

5:10 Paper 652g: Computational Search of Improved Homogeneous Catalysts for the Buchwald-Hartwig Amination Reaction — ***Roberto Schimmenti**, Megha Anand, Jens K. Nørskov*

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(653) Nitrogen Chemistry: Electrocatalytic N2 reduction

Thursday, Nov 17, 3:30 PM
Phoenix Convention Center, N-127C

Huiyuan Zhu, Chair
Nirala Singh, Co-Chair

Sponsored by: Catalysis

3:30 Paper 653a: Techniques for the Examination of Aqueous and Nonaqueous Electrocatalytic N_2 Reduction — ***Adam Nielander**, Sarah Blair, Valerie Niemann, Peter Benedek, Eric McShane, Matteo Cargnello, Thomas Jaramillo*

3:48 Paper 653b: Design of Multinary Electrocatalysts for Selective Nitrogen Reduction to Ammonia — ***Nick Singstock**, Charles B. Musgrave*

4:06 Paper 653c: Evolution of the Solid-Electrolyte Interphase Formed during the Lithium-Mediated Electrochemical Ammonia Synthesis Reaction — ***Eric McShane**, Matteo Cargnello*

4:24 Paper 653d: Advanced Analytical Chemistry Allows Robust Catalyst Verification for Electrochemical N_2 Reduction — ***Weilai Yu**, Katharina Brinkert, Nathan Dalleska, Nathan S. Lewis, Harry Gray*

4:42 Paper 653e: Electrocatalytic Synthesis of Ammonia on Composite Bimetallic Nitride-Perovskite Oxide Soec Cathode — ***Matthew Ferree**, Seval Gunduz, Jaesung Kim, Anne Co, Umit Ozkan*

5:00: Intermission

5:25 Paper 653f: Improvement of Nitrogen Reduction Reaction Via the Proton Transfer on Metal Oxide Catalysts — ***Chi-Ho Lee**, Silabrata Pahari, Joseph Kwon*

5:43 Paper 653g: Enhancing the Nitrogen Reduction Reaction Activity of Ti_2n Nitride Mxene through pH and Electrolyte Selection — ***Denis Johnson**, Abdoulaye Djire*

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(654) Reaction Engineering and Kinetics for Combustion, Pyrolysis & Emissions

Thursday, Nov 17, 3:30 PM
Phoenix Convention Center, N-128B

Bihter Padak, Chair
Manjiri Moharir, Co-Chair
Erdem Sasmaz, Co-Chair

Sponsored by: Reaction Engineering

3:30: Break

3:45 Paper 654a: Automated Generation of Chemical Kinetic Reaction Mechanisms for Combustion of Large Alkanes — ***Venus Amiri***, *Rubik Asatryan, Mark Swihart*

4:00 Paper 654b: Effect of Nitrogen Oxide on the Reactivity of Cu-Mn Oxygen Carrier for Chemical Looping with Oxygen Uncoupling — ***Bihter Padak***, *Turna Barua*

4:15 Paper 654c: Towards Prediction of Ash Deposition Rates from Combustion of a Wide Variety of Fossil and Biomass Solid Fuels. — ***Jost Wendt***, *Xiaolong Li*

4:30 Paper 654d: DFT Study of H_2s Binding on Cu_2o Oxygen Carrier for Chemical Looping with Oxygen Uncoupling (CLOU) — ***Madeline Talebi***, *Bihter Padak*

4:45 Paper 654e: Continuous Compositional Analysis of Emission Streams Using Online Process Analyzers. — ***Avery Brown***, *Eric G. Schmidt, Paul Cammarata, Roger Bustos, Daniel Beery*

5:00 Paper 654f: A DFT Study of so_2 Binding on $CuMn_2O_4$ Oxygen Carrier for Chemical Looping with Oxygen Uncoupling — ***Madeline Talebi***, *Turna Barua, Bihter Padak*

5:15 Paper 654g: Present Status and New Results for Pfas Destruction Chemistry — ***Phillip Westmoreland***, *Hrishikesh Ram, Thomas P. Sadej, C. Claire Murphy*

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(655) Technology Transfer and Industrial-Academic Interfaces

Thursday, Nov 17, 3:30 PM
Phoenix Convention Center, N-127A

Sarika Goel, Chair
Joshua Schaidle, Co-Chair
Brandon O'Neill, Co-Chair

Sponsored by: Catalysis

3:30 Paper 655a: Decarbonizing the Skies – Technology Development for Sustainable Aviation Fuel — ***Derek Vardon***

3:55 Paper 655b: Anything to SAF - Innovations and the Challenges Ahead — ***Eseoghene Jeroro***

4:20 Paper 655c: Renewable Methanol Conversion to Lower Emission Fuels and Sustainable Chemicals — ***Lei Zhang***

4:45 Paper 655d: Scaling up Single-Step Carbon Dioxide Conversion Technology for Sustainable Products — ***Stafford Sheehan***

5:10 Paper 655e: SAF-Prometheus Fuels — ***Rob McGinnis***

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(656) Machine Learning for Soft Materials II

Thursday, Nov 17, 3:30 PM
Phoenix Convention Center, N-222B

Nicholas Jackson, Chair
Michael Webb, Co-Chair
Pin-Kuang Lai, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

3:30: Introductory Remarks

3:35 Paper 656a: A New Computational-Experimental Screening Methodology Identifies More Effective Solvents for CO_2 Capture — ***Frederick de Meyer***, *Alexey Orlov, Christophe Coquelet, Xavier Rozanska*

3:50 Paper 656b: Characterization of Chemoresponsive Liquid Crystals Using Topological Descriptors and Machine Learning — ***Shengli Jiang***, *Nanqi Bao, Alexander Smith, Nicholas L. Abbott, Victor Zavala*

4:05 Paper 656c: Physics-Informed Deep Neural Networks for Predicting Fluid Flow in Complex Porous Materials — ***Serveh Kamrava***, *Muhammad Sahimi*

4:20: Break

4:30 Paper 656d: Simulation of Neutron Dark Field Interferometry Data in Hierarchical Materials Using Small Angle Scattering Models — ***Caitlyn Wolf***, *Youngju Kim, Anis Ben Said, Sarah Robinson, Ryan P. Murphy, M. Cyrus Daugherty, Michael Huber, David L. Jacobson, Jacob LaManna, Nikolai Klimov, Paul Kienzle, Peter Bajcsy, Daniel S. Hussey, Katie Weigandt*

4:45 Paper 656e: Developing an ML Algorithm to Predict the Aqueous Solubility of Polymers and Organic Compounds — ***Arash Tayyebi***, *Ali Alshami*

5:00: Break

5:15: Intermission

5:25 Paper 656g: Machine Learning for the Discovery of Molecular Recognition Based on Single-Walled Carbon Nanotube Corona-Phases — ***Xun Gong***, *Nicholas J Renegar, Retsef Levi, Michael Strano*

5:40 Paper 656h: Accelerated Discovery of Novel Ionic Liquid Cations Using a Continuous Latent Space Representation of Chemical Space — *Pratik Dhakal*, ***Jindal Shah***

5:55 Paper 656i: Context-Aware Representations from Deep Learning for Antibody Design — ***Sai Pooja Mahajan***, *Jeffrey J. Gray*

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(657) Applied Math for Energy and Environmental Applications

Thursday, Nov 17, 3:30 PM
Phoenix Convention Center, W-101B

Apoorva Sampat, Chair
Jin Wang, Co-Chair
Davood Babaei Pourkargar, Co-Chair

Sponsored by: Applied Mathematics and Numerical Analysis

3:30 Paper 657a: A Cellular Automata Framework for Porous Electrode Reconstruction and Ion Transport Simulation — ***Jindong Dai***, *Chi Zhai, Haichao Lv, Jiali Ai, Wei Sun, Yongzhong Liu*

3:49 Paper 657b: High-Speed Growth of Crystalline Wafers for Solar Cells — *Eyan Noronha*, ***Erik Ydstie***

4:08 Paper 657c: Discrete Element Method Model Calibration Using High-Speed Videos and Computer Vision for the Mechanochemical Grinding of Plastic Waste — ***Elisavet Anglou***, *Yuchen Chang, William Bradley, Carsten Sievers, Fani Boukouvala*

4:27 Paper 657d: Developing Optimization Framework for Sustainable Co-Production of Food and Energy — ***Varsha Varsha***, *Mohit Tawarmalani, Margaret W Gitau, Rakesh Agrawal*

4:46 Paper 657e: Using LP-Based Heuristics for Solving Large-Scale Integer Problems — ***Iiro Harjunkoski***

5:05 Paper 657f: Two-Stage Robust Optimization for Alternating Current Optimal Power Flows with Renewables Uncertainty — ***Jason Sherman***, *Carl Laird, Chrysanthos Gounaris*

5:24 Paper 657g: Designing Thermal Energy Storage through Dynamic Optimization Using Process Data — ***Caroline S. M. Nakama***, *Brage R. Knudsen, Agnes C. Tysland, Johannes Jäschke,* ***Zawadi Ntengua Mdoe***

5:43 Paper 657h: Optimal Design of Solar Systems for Decarbonizing Industrial Process Heat Applications — *Sloane Putnam, Justin Rastinejad,* ***Matthew Stuber***

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(658) Planning, Scheduling, Supply Chain and Logistics - II

Thursday, Nov 17, 3:30 PM
Phoenix Convention Center, W-101C

Philip Tominac, Chair
Styliani Avraamidou, Co-Chair

Sponsored by: Systems and Process Operations

3:30 Paper 658a: Diagnosis of Linear Programming Supply Chain Optimization Models: Minimizing Changes for New Parameter Values — ***Sitoshna Jatty***, *Niharika Singh, Ignacio Grossmann, Leonardo Salsano de Assis, Christos Galanopoulos, Bianca Springub, Nga Tran*

3:48 Paper 658b: A Generic Unit-Specific Event-Based Mathematical Formulation for Short-Term Scheduling Multipurpose Batch Plants — ***Dan Li***, *Nikolaos Rakovitis, Taicheng Zheng, Jie Li*

4:06 Paper 658c: Reactive Optimization of Supply Chain Networks Under Disruptions — ***Daniel Ovalle**, Ignacio Grossmann, Carl Laird, Yixin Ye, Kyle Harshbarger, Scott J. Bury*

4:24 Paper 658d: Strengthening Production Scheduling Formulations By Incorporating Record Keeping Variables — ***Nathan Adelgren**, Christos T. Maravelias*

4:42 Paper 658e: Data-Driven Robust Optimization Approach for Scheduling Oil Pipeline Systems — *Amir Baghban, **Pedro Castro**, Fabricio Oliveira*

5:00 Paper 658f: Extensions to the Guaranteed-Service Model for Safety Stock Positioning in Industrial Environments — *Victoria G. Achkar, **Braulio Brunaud**, Hector Perez, Rami Musa, Carlos Méndez, Ignacio Grossmann*

5:18 Paper 658g: Optimal Design and Operation of CO_2 Transportation and Storage Infrastructure for Industrial Clusters — ***Jude O. Ejeh**, Sergey Martynov, Solomon F. Brown*

5:36 Paper 658h: Capacity Planning Considering Both Large-Scale Conventional Facility and Small-Scale Modular Device for Shale Gas Water Management — ***Kaiyu Cao**, Niranjan Sitapure, Joseph Kwon*

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(659) Sustainable Process Synthesis, Design and Intensification

Thursday, Nov 17, 3:30 PM
Phoenix Convention Center, W-101A

Yuhe Tian, Chair
Maria Papathanasiou, Co-Chair

Sponsored by: Systems and Process Design

3:30 Paper 659a: An Integrated Approach to Maximize Process and Strain Efficiency in Biochemical Processes:the Case of Bioplastics Production and Muconic Acid. — *Stefanos Xenios, Daniel Weilandt, Vassily Hatzimanikatis, Ljubisa Miskovic, **Antonios Kokosis***

3:51 Paper 659b: An Integrated Set of Methods, Algorithms and Software Components for Sustainable Process Design — ***Orakotch Padungwatanaroj**, Jakkraphat Koncharoenkitkul, Raksina Promphan, Mario Eden, Rafiqul Gani*

4:12 Paper 659c: Optimisation of Solar-Aided Hydrogen Production Process Integrated Carbon Capture Using Methyl Diethanolamine/Piperazine with Carbon Dioxide Utilisation — ***Wanrong Wang**, Nan Zhang, Jie Li*

4:33 Paper 659d: Digitalization and Optimization Boost Decarbonization: Accelerating Net Zero from the Perspective of Carbon Capture and Utilization — ***Zhimian Hao**, Magda Barecka, Alexei A. Lapkin*

4:54 Paper 659e: Modular Process Intensification Synthesis for Membrane-Based Reactive Separation Systems Towards Sustainable Hydrogen Production — ***Yuhe Tian**, Ayooluwa Akintola*

5:15 Paper 659f: Techno-Economic and Life Cycle Assessment of an Electro- and Bio-Catalytic Carbon Upgrade Process — ***Isaiah Chen**, Andrew W. Ruttinger, Sarah M. Jordaan, Paulette Clancy*

5:36 Paper 659g: Cryogenic Energy Storage: Design, Techno-Economic Analysis, and Integration with Power Plants and Renewables — ***Akhilesh Gandhi**, Manali S. Zantye, M M Faruque Hasan*

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(660) Development of Intermolecular Potential Models

Thursday, Nov 17, 3:30 PM
Phoenix Convention Center, N-222C

Neeraj Rai, Chair
Andrew Paluch, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

3:30 Paper 660a: Molecular Simulations of Vapor–Liquid Equilibrium of Isocyanates — ***Alina Emelianova**, Gennady Gor*

3:46 Paper 660b: High-Dimensional Neural Network Potentials for Molecular Dynamics Simulations of Crystal Thermodynamics and Phase Transition — ***Hao Deng**, Bin Liu*

4:02 Paper 660c: Development of an Atomistic Forcefield for Peptoids — ***Rakshit Jain**, Carol Hall, Erik Santiso*

4:18 Paper 660d: Intelligent Algorithms for the Design of Rare-Earth Metal Forcefields — ***Kevin Hinkle***

4:34 Paper 660e: Development of High-Accuracy Semiempirical Models with a Minimal Training Set — ***C. Huy Pham**, Rebecca Lindsey, Laurence E. Fried, Nir Goldman*

4:50: Break

5:06 Paper 660g: The Interface Force Field for Halide Perovskites and First Applications to Materials for Solar Energy Harvesting — ***Barbara Morales**, **Hendrik Heinz***

5:22 Paper 660h: Parametrization of Coarse-Grained Models for Real Polymer Systems to Simulate Block Copolymers — ***Sahar Zenoozi**, Peter J. Ludovice, Clifford Henderson*

5:38 Paper 660i: The Open Force Field v2.0 and Extensions to Biopolymers — *John Chodera, Michael K. Gilson, David L. Mobley, **Michael Shirts***

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(661) Design and Optimization of Integrated Energy Systems

Thursday, Nov 17, 3:30 PM
Phoenix Convention Center, N-225B

Alexander Dowling, Chair
Dhabia Al-Mohannadi, Co-Chair
David Miller, Co-Chair

Sponsored by: Climate Change

3:30 Paper 661a: *Generalized Disjunctive Programming* (GDP) Model for the Optimal Capacity Planning of Reliable Power Generation Systems — ***Seolhee Cho**, Ignacio Grossmann*

3:51 Paper 661b: Lessons from an Integrated Optimisation Model of the UK Power, Heating, and Hydrogen Sectors — ***Matthias Mersch**, Christos N. Markides, Niall Mac Dowell*

4:12 Paper 661c: GHG Emissions Reduction By Optimizing Design and Operation of Cross-Sector Integrated Energy Systems: Civic and Industrial Sectors — ***Ruonan Li**, **Vladimir Mahalec***

4:33 Paper 661d: Decarbonising Residential Heating with Uncertain Fuel Costs: A Whole-System Value Chain Optimisation — ***Jennifer Penman**, Sheila Samsatli*

4:54 Paper 661e: Long-Term Expansion Planning of an Integrated Power and Energy Carrier Generation System: A Tailored Decomposition Algorithm — ***Iasonas Ioannou**, Ignacio Grossmann, Gonzalo Guillén-Gosálbez*

5:15 Paper 661f: A Dynamic Optimization Model for Minimizing the Cost of Low-Carbon Industrial Clusters — *Mohamed Lameh, **Dhabia Al-Mohannadi**, Patrick Linke, Yasir Ibrahim*

5:36 Paper 544f: Optimal Deployment Under Uncertainty of Negative Emissions Technologies in the European Union Power System — ***Valentina Negri**, Ignacio Grossmann, Gonzalo Guillén-Gosálbez*

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(662) Waste Plastic - Recycle, Reuse and Remediation Strategies II

Thursday, Nov 17, 3:30 PM
Phoenix Convention Center, N-225A

Jeffrey Seay, Chair
Amy E. Landis, Co-Chair
Robert Peters, Co-Chair

Sponsored by: Solid and Hazardous Waste

3:30 Paper 662a: Microbial Upcycling of Thermally Oxo-Degraded Plastic Wastes — ***Efrain Rodriguez-Ocasio**, Jessica Brown, Robert Brown, Mark Blenner, Laura R. Jarboe*

3:48 Paper 662b: Polymer Melt Dynamics on Catalyst Surfaces Using Replica Exchange Molecular Dynamics Simulations — ***Mehdi Zare***, *Dionisios Vlachos, Stavros Caratzoulas*

4:06 Paper 662c: Analysis of Solvent-Assisted Chemical Recycling of Plastics Using a Superstructure Optimization Approach — ***Austin Lehr***, *Emmanuel Aboagye, John Chea, Jake Stengel, Kirti Yenkie, Pahola Thathiana Benavides*

4:24 Paper 662d: Computational Insights into the Thermodynamic Properties of Circular Polymers — ***Sai Phani Kumar Vangala***, *Alexander Shaw, Linda Broadbelt*

4:42 Paper 662e: Additive-Induced Catalyst Poisoning in Polyolefin Hydrocracking — ***Zachary Hinton***, *Pavel Kots, Dionisios Vlachos, Thomas H. Epps, III, LaShanda Korley*

5:00 Paper 662f: Chemical Deconstruction of Polyethylene Terephthalate (PET) into Soluble, Nitrogen-Enriched Compounds for Microbial Upgrading — ***Muhammad Aamir Bashir***, *Libby Umlor, Laura Schaerer, Stephen Techtmann, Rebecca Ong*

5:18 Paper 662g: Upcycled Polyvinyl Chloride (PVC) Electrospun Nanofibers Fabricated from Waste PVC for Water Treatment — ***Atta Ur Razzaq***, *Milad Esfahani*

5:36 Paper 662h: Effective Depolymerization of Polyethylene Plastic Wastes Under Hydrothermal and Solvothermal Liquefaction Conditions — ***Yixin Liu***, ***Kapil Chandra Akula***, ***Alexa Sanchez***, *Shuguang Deng*

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(663) Biobased and Bioderived Processes for Value Added Chemicals and Advanced Materials

Thursday, Nov 17, 3:30 PM
Phoenix Convention Center, N-125B

Jin Ryoun Kim, Chair
Hyunmin Yi, Co-Chair

Sponsored by: Bioengineering

3:30 Paper 663a: A New Class of Xylose-Based Green Solvents Produced from Renewable Biomass — ***Anastasia Komarova***, *Zezhong Li, Jeremy Luterbacher*

3:48 Paper 663b: Recombinant Production and Purification of Green Fluorescent Protein (GFP)-Fused Metal Binding Protein for Palladium Nanoparticle Synthesis — ***Shadrach Ibinola***, *Hazim Aljewari, Imann Mosleh, PhD, Robert Beitle, Rita Tejada Vaprio*

4:06 Paper 663c: Renewable Bio-Graphene Synthesis and Its Application As an Anti-Corrosive Coating — ***Suriya Narayanan Ramasubramanian***, *Hema Ramsurn, Gabriel LeBlanc*

4:24 Paper 663d: Thermoplastic Degradation By Yellow Mealworm Gut Microbial Communities and Isolates — *Lummy Monteiro, Jyoti Singh, Ross Klauer, Kevin Solomon,* ***Mark Blenner***

4:42 Paper 663e: Genome Mining Unveils Class of Ribosomal Peptides with Two Amino Termini — ***Hengqian Ren***, *Shravan R. Dommaraju, Chunshuai Huang, Haiyang Cui, Yuwei Pan, Marko Nesic, Lingyang Zhu, David Sarlah, Douglas A. Mitchell, Huimin Zhao*

5:00 Paper 663f: Identifying the Genetic Mechanisms of Diatom Silicification for the Production of Novel Biomaterials — ***Hugh Purdy***, *Michelle O'Malley*

5:18 Paper 663g: Dose-Controllable Long-Term Drug Delivery Implant — ***Yoonjee Park***, *Xingyu He, Zheng Yuan*

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(664) Diagnostic Technologies for Clinical Applications

Thursday, Nov 17, 3:30 PM
Phoenix Convention Center, N-125A

Piyush Jain, Chair
Chang Liu, Co-Chair

Sponsored by: Bioengineering

3:30: Break

3:48 Paper 664a: A Low-Cost Paper-Based Sample Preparation Module to Lyse Bacterial Cells and Extract Genomic DNA Using Isotachophoresis — ***Shruti Soni***, *Bhushan Toley*

4:06: Break

4:24 Paper 664c: Colorimetric Assay for Pneumonia Screening Via the Volatile Organic Breath Biomarker, Heptane — ***Bailey Doucette***

4:42 Paper 664d: Leveraging the Ordered Packing of Spherocytes As a Potential Diagnostic — ***Logan Piegols***, *Tobias Dwyer, Sharon Glotzer, Omolola Eniola-Adefeso*

5:00 Paper 664e: Excitation-Scanning Hyperspectral Imaging Technologies for Multilabel Cellular Imaging — ***Silas Leavesley***, *Naga Srilakshmi Annamdevula, Madison Howard, Craig Browning, Marina Parker, William Oswald, Andrea Britain, C. Michael Francis, Na Gong, Thomas Rich*

5:18 Paper 664f: Vapor Biomarker Analysis for Precision Healthcare: From Benchtop to Wearable — ***Xudong Fan***

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(665) Systems Biology of Development and Cancer

Thursday, Nov 17, 3:30 PM
Phoenix Convention Center, N-126B

Gregory Reeves, Chair
Jason E. Shoemaker, Co-Chair
Whitney Stoppel, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

3:30 Paper 665a: Differential Gene Expression Analysis of Primary Human Hepatocytes and iPSC-Hepatocyte like Cells By RNA Seq — ***Neeti Gandhi***, *Kyle Akers, Lauren Wills, T. M. Murali, Padmavathy Rajagopalan*

3:48 Paper 665b: Transcription of Proximal RNAs Can Regulate Gene Expression By Modulating Transcriptional Condensate Dynamics — ***Pradeep Natarajan***, *Krishna Shrinivas, Halima Schede, Jonathan E. Henninger, Ozgur Oksuz, Arup K. Chakraborty, Mehran Kardar, Richard A. Young, Phillip A. Sharp*

4:06 Paper 665c: Dissecting the Role of a Tumor Suppressor Protein in Enabling Highly-Efficient Reprogramming — ***Adam Beitz***, *Brittany Lende, Kate Galloway*

4:24 Paper 665d: Short Chain Fatty Acid Influence on Normal and Estrogen Deficient Bone Remodeling — ***Carley V. Cook***, *Brenda J. Smith, Ashlee Ford Versypt*

4:42 Paper 665e: An Optimal Regulatory Grammar for Dynamic Gene Control in Space and Time — *Sahla Syed,* ***Bomyi Lim***

5:00 Paper 665f: Modeling Supercoiling-Dependent Feedback As a Transcriptional Coordinator to Understand and Engineer Biological Circuits. — ***Christopher Johnstone***, *Kate Galloway*

5:18 Paper 665g: Invited Talk: Biomechanics of Epithelial Tissue Homeostasis, Collapse, and Eversion — *Vani Narayanan, Purboja Purkayastha, Bo Yu,* ***Richard Dickinson***, *Daniel Conway, Tanmay Lele*

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(666) Chemical Modifications and Processing of Biomaterials II

Thursday, Nov 17, 3:30 PM
Phoenix Convention Center, N-228A

Zhaohui Tong, Chair

Sponsored by: Forest and Plant Bioproducts Division

3:30 Paper 666a: Hydrophobic and Water-resistant Lignocellulosic Packaging Materials Enabled by Metal Ion Modification — ***Xuefeng Zhang***, *R.M. Oshani Nayanathara*

4:00 Paper 666b: To Enhance Adhesion Property of Soy Protein Adhesive By Base-Solvents Modified Guayule Resin — ***Sarocha Pradyawong***, *Kimberly Ogden*

4:30 Paper 666c: Hydrolytically Stable Films from 3-Aminopropyl Triethoxysilan (APTES) Modified Cellulose Nanocrystals — ***Sadat Kamal Amit***, *Diego Gómez Maldonado, Maria Soledad Peresin, Virginia Davis*

(667) Division Plenary: Valorization of Waste plastics including Ocean Plastics along with Agro-residues/Forestry waste for Sustainable Biocomposites (Invited Talks)

Thursday, Nov 17, 3:30 PM
Phoenix Convention Center, N-229AB

Amar K. Mohanty, Chair
Manjusri Misra, Co-Chair

Sponsored by: Forest and Plant Bioproducts Division

3:30 Paper 667a: The Drive for Greener Materials and Sustainability Leadership — ***Debbie F Mielewski***

4:00 Paper 667b: Tree Bark-Derived Lignin Containing Nanocellulose Fibrils for Enhancing Performance of Plastic Composites — ***Ning Yan***

4:30 Paper 667c: Fabrication of Lignocellulose-Based Materials for Environmental, Energy, and Packaging Applications — ***Xuejun Pan***

5:00 Paper 667d: Value Addition of Waste Plastics through Upcycling for a Sustainable Future — ***Amar K. Mohanty***

5:30 Paper 667e: Refined Chemicals and Carbonaceous Materials Derived from Biomass Pyrolysis — ***Yaseen Elkasabi***

(668) Hydrogel Biomaterials III: Design and Characterization

Thursday, Nov 17, 3:30 PM
Phoenix Convention Center, N-121B

Amir Sheikhi, Chair
Marjan Rafat, Co-Chair
Mai Ngo, Co-Chair
Mark Tibbitt, Co-Chair

Sponsored by: Biomaterials

3:30 Paper 668a: Durability and Lubricity of Photografted Zwitterionic Hydrogel Coatings — ***Adreann Peel***, *Allan Guymon*

3:45 Paper 668b: Engineering Hydrogel Biomaterials with Tunable Mechanics and Proteolytic Stability Using Peptide Stereochemistry — ***Israt Jahan Duti***, *Jonathan Paul, Emma Laudermilch, Rachel Letteri*

4:00 Paper 668c: Supramolecular Reinforcement of Polymer–Nanoparticle Hydrogels for Modular Material Design — ***Giovanni Bovone***, *Elia A. Guzzi, Stéphane Bernhard, Tim Weber, Dalia Dranseikiene, Mark Tibbitt*

4:15 Paper 668d: Mapping of Collagen and Hyaluronic Acid Hydrogel Properties to Functional Responses — ***Paulina Babiak***, *Mazin Hakim, Qinghua Xu, Wesley Holt, Jessica Torres, Kevin Buno, Ilias Bilionis, Luis Solorio, Julie C. Liu*

4:30 Paper 668e: Anisotropic Chitosan Hydrogels with Multi-Length-Scale Layered Structures Via Directional Drying — ***Wei Li***, *Qingye Liu*

4:45 Paper 668f: Synthesis, Characterization, and Analysis of Free Radical Scavenging Thermo-Responsive Hydrogels with Therapeutic Capabilities — ***Samina Yasmeen***

5:00 Paper 668g: Non-Equilibrium Characterization of Injectable Polymer Nanoparticle Hydrogels — ***Noah Eckman***, *Abigail Grosskopf, Grace Jiang, Julie Baillet, Eric A. Appel*

5:15 Paper 668h: Using Magnetic Fields to Control Fiber Alignment within Fiber-Hydrogel Composites — ***Grace Schwarz***, *Julianne Holloway*

(669) Materials for Quantum Science

Thursday, Nov 17, 3:30 PM
Phoenix Convention Center, N-121C

Matthew Crane, Chair
William Tisdale, Co-Chair

Sponsored by: Electronics and Photonics

3:30 Paper 669a: TBD — ***Jennifer Dionne***

4:00 Paper 669b: Understanding Structure-Property Relationship of Metal-Organic Frameworks and Their Efficiency on Second Harmonic Generation — ***Sanoj -***, *Rubén Fritz, Felipe Herrera, Yamil Colón*

4:15 Paper 669c: Chiral Inorganic Hedgehogs with Birefringence — ***Prashant Kumar***, *Nicholas Kotov*

4:30 Paper 669d: Colloidal Synthesis and Optical Characterization of Chalcogenide Non-Linear Optical (NLO) Particles, $Na_2Ba_7Sn_4S_{16}$ (NBTS) — ***Alexander Jess***, *Calvin Fai, Charles Hages*

4:45 Paper 669e: Extending Spin-Dephasing Lifetimes in Metal-Halide Perovskites By Morphology Engineering — ***Matthew Crane***, *Laura Jacoby, Daniel Gamelin*

5:00 Paper 669f: Quantum Dot Doped Lead Halide Perovskites for Ionizing Radiation Detection — ***Ashley M. Conley***, *Ephraiem Sarabamoun, Katelyn Dagnall, Lucy U. Yoon, Seung-Hun Lee, Joshua Choi*

5:15 Paper 669g: Benzobisthiadiazole-Based High-Spin Donor-Acceptor Conjugated Polymers with Localized Spin Distribution — ***Md Abdus Sabuj***, *Chandra Sarap, Md Masrul Huda, Neeraj Rai*

5:30 Paper 669h: The Synthesis and Engineering of Two-Dimensional Janus Quantum Layers — ***Sefaattin Tongay***

(670) Polymer Thermodynamics and Self-Assembly: Polymer-Molecular Interactions

Thursday, Nov 17, 3:30 PM
Phoenix Convention Center, N-122B

Reza Foudazi, Chair
Douglas Tree, Co-Chair
Zhe Qiang, Co-Chair
S. Eileen Seo, Co-Chair
Ian Hosein, Co-Chair
Melody Morris, Co-Chair

Sponsored by: Polymers

3:30 Paper 670a: Understanding the Spontaneous Segregation of Bottlebrush Additives to Surfaces and Interfaces — *Dongjoo Lee, Nilesh Charpota, Travis Law, Gila E. Stein,* ***Rafael Verduzco***

4:00 Paper 670b: Influence of Ionic Liquids on Polymer Nanostructure Formed within Lyotropic Liquid Crystalline Templates — ***Alexandros Kotsiras***, *Allan Guymon*

4:15 Paper 670c: Fast Multi-Stimuli-Responsive Nanoporous Hydrogels Produced from Polymerization of Lyotropic Liquid Crystals — ***Younes Saadat***, *Kyungtae Kim, Reza Foudazi*

4:30 Paper 670d: Molecular Dynamics Study of Hydrophilic-Hydrophobic Diblock Copolymer Self-Assembly: Phase Diagram, Vesicle Morphogenesis, and Shear Flow Dynamics — *Senyuan Liu,* ***Radhakrishna Sureshkumar***

4:45 Paper 670e: Effect of Monomer Sequence on Polymer Solution Phase Behavior — ***Lauren Taylor***, *Rodney Priestley, Richard A. Register*

5:00 Paper 670f: On the Thermodynamic Consistency of Phase-Field Models of Polymeric Solutions — ***Rami Alhasan***, *Douglas Tree*

5:15 Paper 670g: Co-Solvency Induced Micro- and Macro-Phase Behavior of Polymers in Mixed Solvents — *Xiangyu Zhang,* ***Dong Meng***

5:30 Paper 670h: Field-Theoretic Modeling of Neutral Solvent Effects on Diblock Copolymer Self-Assembly — ***Thomas Habte***, *Andrew Spakowitz*

5:45 Paper 670i: Using Periodic Dynamic Polymers to Form Ordered Supramolecular Structures — ***Christopher B. Cooper***, *Zhenan Bao*

(671) Polymer Thin Films, Confinement, and Interfaces II

Thursday, Nov 17, 3:30 PM
Phoenix Convention Center, N-122A

Kathleen McEnnis, Chair
Julie Albert, Co-Chair
Jean-Francois Louf, Co-Chair
Rong Yang, Co-Chair

Sponsored by: Polymers

3:30 Paper 671a: Mechanics of Ultra-Thin Polymer Glasses — ***Alfred Crosby***

4:00 Paper 671b: Drying-Induced Bending of Hydrogel Disks — ***Jean-Francois Louf***, *Haohui Zhang, Marykate Neff, Yuhang Hu, Sujit Datta*

4:15 Paper 671c: Effect of Surface Stress on Roughness and Adhesion of Soft Solids — ***Preetika Karnal***, *Chung-Yuen Hui, Anand Jagota*

4:30 Paper 671d: Poroelastic Mechano-Sensing Soft Robots — ***Tofayel Ahammad Ovee***, *Jean-Francois Louf*

4:45 Paper 671e: Lubricated Friction of Soft Solid Surfaces: Transition from Elastohydrodynamic to Mixed Regime — ***Hao Dong***, *Nichole Moyle, Haibin Wu, Constantine Khripin, Chung-Yuen Hui, Anand Jagota*

5:00 Paper 671g: Glass Transition Temperature in PLGA Nanoparticles — ***Guangliang Liu***, *Kathleen McEnnis*

5:15: Break

5:30 Paper 671i: Ultra-High Dielectric Strength and Capacitive Energy Density in Ultrathin Glassy Polymer Films — ***Maninderjeet Singh***, *Dharmaraj Raghavan, Nihar Pradhan, Alamgir Karim*

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(672) Advancements in Particle Engineering and Material Sciences in Pharmaceutical Process Development I

Thursday, Nov 17, 3:30 PM
Phoenix Convention Center, N-123

Parind Desai, Chair
Srivatsan Ramesh, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

3:30 Paper 672a: Control of Crystal Morphology through Process Parameter Optimization Guided By 2d PBM — ***Brian Seifried***, *Tamar Rosenbaum, John Gamble, Joshua Engstrom, Ulrich Schacht, Yash Melkeri, Niall Mitchell*

3:51 Paper 672b: Introducing Contcarsim, a Benchmark Simulator for Design and Control of Continuous Integrated Filtration-Drying of Crystallization Slurries — ***Francesco Destro***, *Massimiliano Barolo, Zoltan Nagy*

4:12 Paper 672c: Equipment Optimization for Cryogenic Particle Formation Correlating Experimental and Model Results — ***Howard Stamato***, *Nima Yazdanpanah, Jorge Lopez, Russel Carson, Edwin Amoro, Elliott Bay, Jason Antunovich*

4:33 Paper 672d: Non-Classical Crystallisation to Decrease the Impurity Transfer Kinetics during the Crystal Growth of Curcumin from Their Impure Solutions — ***Mahmoud Ranjbar***, *Gavin Walker, Vasanth Kumar Kannuchamy*

4:54 Paper 672e: Development of a Crystallization Process to Prevent Oiling and Optimize Physical Properties of a Drug Substance — ***Peter Galebach***, *Zachary Garlets, Andrew Werneth, Melda Sezen-Edmonds*

5:15 Paper 672f: Investigating the Effect of Droplet Confinement and Porous Confinement on the Formation of Carbamazepine Polymorphs — ***Alice Parkes***, *Ahmad Ziaee, Gavin Walker, Emmet O'Reilly*

5:36 Paper 672g: Engineering Theranostic Superparamagnetic Nanoparticles for Hyperthermia and Magnetic Particle Imaging Using a Quality-By-Design Approach — ***Shaquib Rahman Ansari***, *Ioannis Katsaros, Michelle Åhlén, Christel A.S. Bergström, Peter Svedlindh, Carlos Rinaldi-Ramos, Alexandra Teleki*

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(673) Modeling solubility, dissolution, permeability and drug delivery

Thursday, Nov 17, 3:30 PM
Phoenix Convention Center, N-122C

Yuriy Abramov, Chair
Ebenezer Ojo, Co-Chair
Daniel Hallow, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

3:30 Paper 673a: Exploring the Effects of Equipment Operational Defects on the Dissolution Performance in USP Apparatus 1 — ***Eric Murphy***, *Julie Spence, Daniel Reinders, Eric Nielsen, Susan George, Yi Gao, Ann M. Czyzewski, Nandkishor Nere*

3:55 Paper 673b: First Principles and Cheminformatics Based in-Silico Tools for Physical Property Prediction Towards Informed Process Development — ***Sharad Maheshwari***, *Pelin Su Bulutoglu, Eric Murphy, Kushal Sinha, Akshay Korde, Moussa Boukerche, James Marek, Ryan Ellis, Manish Kelkar, Daniel Pohlman, Richard Hong, Nathan Abraham, Rajni Miglani Bhardwaj, Jeremy Henle, Nandkishor Nere*

4:20 Paper 673d: Predicting the Solubility of Amino-Acid Mixtures with the SAFT-γ Mie Group-Contribution Method — ***Ahmed Alyazidi***, *Andrew J. Haslam, George Jackson, Amparo Galindo*

4:45 Paper 673e: A Mathematical Model to Predict the Drug Release Profile in a Single-Layered Osmotic Controlled Release Tablet — ***Bhawana Tomar***, *Mahesh S. Tirumkudulu, Sweta Manthena, Weili Yu, Alfred Berchielli, Pankaj Doshi*

5:10 Paper 673g: An Adaptive Sampling Surrogate Model for Mixing Time Prediction and Mixing Characterization — *Maryam Medghalchi*, ***Saeed Jafari Kang***, *Iman Mirzaee, Joao de Faria, Fabrice Schlegel, Pablo A. Rolandi*

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(674) Chromatographic Separations and SMB

Thursday, Nov 17, 3:30 PM
Phoenix Convention Center, N-131C

Balamurali Sreedhar, Chair
Arvind Rajendran, Co-Chair

Sponsored by: Adsorption and Ion Exchange

3:30: Welcoming Remarks

3:35 Paper 674a: Safer Solvents for Active Pharmaceutical Ingredients Purification Using Column Chromatography — ***Christian Ayafor***, *Toren Burton, Gregory Morose, Hsi-Wu Wong*

3:55 Paper 674b: Use of SMB Technology to Extract Oxygenates from Dilute Fermentation Broth — ***Deepak Sharma***

4:15 Paper 674c: Gas-Phase Simulated Moving Bed for Methane/Nitrogen Separation Using a Commercial Activated Carbon — ***Rafael Dias***, *Alexandre Ferreira, Alírio E. Rodrigues, Ana M. Ribeiro*

4:35 Paper 674d: Parameter Estimation for Reactive Chromatography Model By Bayesian Inference and Parallel Sequential Monte Carlo — ***Hikari Sugiyama***, *Yota Yamamoto, Kensuke Suzuki, Tomoyuki Yajima, Yoshiaki Kawajiri*

4:55 Paper 674e: Can a Computer "Learn" Non-Linear Chromatography?: Physics-Based Deep Neural Networks for Chromatographic Separations — ***Sai Gokul Subraveti***, *Zukui Li, Vinay Prasad*, ***Arvind Rajendran***

5:15 Paper 674f: Mechanistic Modeling and Control of Column-Free Continuous Chromatography Process — *Frederik Doerr*, ***Anish Dighe***, *Amos E. Lu, Eben Crawford, Oleg Shinkazh, Richard D. Braatz*

5:35 Paper 674g: Process Modeling and Techno-Economic Optimization of a Moving Bed Contactor for CO_2 Capture Using a Diamine-Appended Metal–Organic Framework — ***Ryan Hughes***, *Goutham Kotamreddy, Debangsu Bhattacharyya, Stephanie Didas, Surya T. Parker, Jeffrey R. Long, Benjamin P. Omell, Michael S. Matuszewski*

5:55: Concluding Remarks

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(675) Fundamentals, Big Data, Machine Learning and High-throughput screening for Bioseparations

Thursday, Nov 17, 3:30 PM
Phoenix Convention Center, N-131B

David Latulippe, Chair
Steve Benner, Co-Chair

Sponsored by: Bio Separations

3:30 Paper 675a: Combinatorial Screening of Ligand-Functionalized Microbeads for Unmethylated and Methylated DNA Binding Application — ***Subhadeep Dutta***, *Tyree Ratcliff, Curt Breneman, Kaushal Rege*

3:51 Paper 675b: Ultrafiltration of Monoclonal Antibodies: Combined Optimization of Formulation Parameters and Process Operating Conditions Under Uncertainty — ***Francesco Rossi***, *Fernanda Cunha, Eduardo Ximenes, Brian D. Bowes, Zhao Yu, Dennis T. Yang, Vincent Corvari, Michael Ladisch, Gintaras Reklaitis*

4:12 Paper 675c: Mechanistic Modeling of Tangential Flow Filtration to Guide Process Development — ***Michael Hartmann***, *Ariella Schwartz, John Welsh, Jennifer Pollard*

4:33 Paper 675g: A New Generation of Materials for Sustainable and Wearable Hemodialysis: Tests and Molecular Screening. — *Thomas Fabiani,* ***Maria Grazia De Angelis***, *Eleonora Ricci, Cristiana Boi, Simone Dimartino*

4:54 Paper 675e: Partitioning and Mass Transport for Continuous Two-Phase Extraction of Viral Vaccines — ***Seth Kriz***, *Rehab Alhajjar, Ethan Burghardt, Christopher Kirschke, Sneha Singh, Pratik Joshi, Caryn Heldt*

5:15 Paper 675f: Advancing Real-Time Live Cell Imaging Technologies to Support the Development of Downstream Purification Processes for Therapeutic Viruses — ***Claire Velikonja***, *Landon Steenbakkers, Ian Gough, Elsa Sorman Paulsson, Christoffer Edlund, Rickard Sjogren, Kalpana Barnes, Brandon Corbett, Prashant Mhaskar, David Latulippe*

5:36 Paper 675d: Multi-Well Device for High-Throughput Screening of Any Flat Sheet Membrane Adsorber — ***Ana Arezina***, *Karina Kawka, Alexandra Jucan, Sarah Arnold, Boyang Zhang, David Latulippe*

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(676) PAT and Process Monitoring in Crystallization Development and Manufacturing

Thursday, Nov 17, 3:30 PM
Phoenix Convention Center, N-131A

Martha Grover, Chair
Hossein Salami, Co-Chair
Matthew McDonald, Co-Chair

Sponsored by: Crystallization and Evaporation

3:30: Welcoming Remarks

3:33 Paper 676a: Development and Application of a Quick Image Analysis Calibration Procedure for in-Situ Crystal Size Measurement — ***Wei-Lee Wu***, *Madeline Mills, Erik Larmore, Ulrich Schacht, Vaso Vlachos, Zoltan Nagy*

4:02 Paper 676b: Characterization and Modelling Reactive Protein Crystallization: Defining the End of a Process — ***Isabella Jul-Jørgensen***, *Ryan Oliver, Anna Carnerup, Krist V. Gernaey, Christian A. Hundahl*

4:31 Paper 676c: Digital Design Framework for the Continuous Crystallization of Diphenhydramine — ***Yash Barhate***, *Hemalatha Kilari, Wei-Lee Wu, Jaron Mackey, Haotang Li, Zoltan Nagy*

5:00 Paper 676d: Process Analytical Technology Controlled Crystallization of Energetic Materials — ***Mouhcine Doukkali***, *Eric Gauthier*

5:29 Paper 676e: Improved Particle Characterisation from in-Line PAT: Comparison of Deep Learning and White-Box Methods — ***Christopher Boyle***, *Cameron Brown, Jan Sefcik, Javier Cardona*

5:58: Concluding Remarks

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(677) Scale-up and Industrial Applications of Adsorption

Thursday, Nov 17, 3:30 PM
Phoenix Convention Center, N-130

Celio Cavalcante Jr., Chair
Armin Ebner, Co-Chair

Sponsored by: Adsorption and Ion Exchange

3:30 Paper 677a: Predicting and Mitigating Retro-Condensation in TSA Dryers Using Aspen Adsorption — ***Robert Broekhuis***, *Pranit S. Metkar*

3:55 Paper 677b: Feasibility Study of Pressure Swing Adsorption (PSA) Processes for CO_2 Capture and H_2 Purification in Blue Hydrogen Processes and Hydrogen Deblending in the Gas Network — *Yan Chen,* ***Hyungwoong Ahn***

4:20 Paper 677c: Variability of Adsorption Properties on HiSiV3000 Individual Pellets — *Stylianos Kalaitzopoulos,* ***Enzo Mangano***, *Stefano Brandani*

4:45 Paper 677d: Controlled Morphology, Post-Synthetic Modification, and Scale-up of MOFs for Direct Air Capture of Carbon Dioxide — ***Xakin Ramirez Isunza***, *Brittany Bonnett, Connor Farrell, Amanda J. Morris, Stephen Martin*

5:10 Paper 677e: Trace Metal Removal By Adsorption for Ultra-High Purity Amines — ***Yujun Liu***, *Towhid Hasan, Xue (Ida) Chen, Jerrod Ruddick, James York, Amarnath Singh*

5:35 Paper 677f: Selective Adsorption of Chlorofluorocarbons(CFC) and Hydrochlorofluorocarbons(HCFC) in Hydrofluorocarbon's (HFC) Using Adsorbent Supported Metal Oxide. — ***Anup Kumar Doraiswamy***

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(678) Surface Engineered and Responsive Membranes

Thursday, Nov 17, 3:30 PM
Phoenix Convention Center, N-132A

Ranil Wickramasinghe, Chair
Ayse Asatekin, Co-Chair
Dona Foster, Co-Chair

Sponsored by: Membrane-Based Separations

3:30 Paper 678a: RO Membranes with Surface Tethered Poly(acrylic acid) Chains for Low Fouling, Ease of Cleaning, Selective Removal and Hydraulic Permeability and Salt Rejection Tunability — ***Yoram Cohen***, *Yian Chen*

3:51: Break

4:12 Paper 678c: Designing, Preparing and Characterizing Alkali Treated Graphitic Carbon Nitride Thin-Film Composites Membranes for Efficient Dye Salty Water Separation. — ***Ameya Tandel***, *Haiqing Lin*

4:33 Paper 678d: Thermo-Responsive Hollow Fiber Membranes for Enhanced Detoxification of Water and Air Pollutants — ***Rollie Mills***, *Thomas Dziubla, J. Todd Hastings, Lindell Ormsbee, Dibakar Bhattacharyya*

4:54 Paper 678e: Electrocoagulation Combined with Electrospun Membranes for Membrane Distillation — ***Yuhe Cao***, ***Ranil Wickramasinghe***

5:15 Paper 678f: Enhancing PFOS Removal and Membrane Permeability By Functionalizing Polyamide Thin-Film Nanocomposite Hollow Fiber Membranes with Mxene Nanosheets — ***Tin Le***, *Elnaz Jamshidi, Majid Beidaghi, Milad Esfahani*

5:36 Paper 678g: Gold Nanoclusters Immobilised Onto Polymer Brushes As Stable Anti-Microbial Surfaces — ***Nidhi Kapil***, *Halan Mohamed, Shanom Ali, Marc-Olivier Coppens*

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(679) Chemical and Catalytic Conversions and Processes for Renewable Feedstocks

Thursday, Nov 17, 3:30 PM
Phoenix Convention Center, N-226B

LiLu Funkenbusch, Chair
Aida Amini Rankouhi, Co-Chair

Sponsored by: Sustainable Biorefineries

3:30 Paper 679a: Remediation of Biomass Pyrolysis Oil Distillate Residues Using Solvent Liquefaction — ***Yaseen Elkasabi***, *Charles A. Mullen*

3:42 Paper 679b: Computational Studies of the Active Sites of Pt and Pt_xCo_y Alloys for Phenol Hydrogenation — ***Isaiah Barth***, *James Akinola, Takaaki Miki, Nirala Singh, Bryan Goldsmith*

3:54 Paper 679c: Catalytic Pyrolysis of Industrial Hemp Biomass for Hydrocarbon Fuels Production — ***Foster Agblevor***, *Myles Bradely, Hamza Abdellaoui, Rachel Criddle, William Corbett*

4:06 Paper 679d: Catalytic Production and Solvent Properties of Furfural-Derived Tetrahydropyran — ***Raka G. Dastidar***, *Panzheng Zhou, Kevin Barnett, Daniel J. McClelland, Reid Van Lehn, George Huber*

4:18 Paper 679e: Epoxidation of Used Cooking Oils Using Heterogeneous Heteropolyacid Catalysts — *Juliana Cardenas, **Alvaro Orjuela**, Benjamin Katryniok, Marcia Araque Marin*

4:30 Paper 679f: On the Influence of Trialkylamine Reduction Strategies in the Direct Hydrogenation of CO_2 to Formic Acid — ***Anouk de Leeuw den Bouter**, Lars Vogels, Esther Vogels, Adeline Miquelot, Pierre Olivier, Camel Makhloufi, John van der Schaaf*

4:42 Paper 679g: Ethanol Conversion to C_{4+} Olefins over Bimetallic Zn-, Cu-, Y-, and La-Containing Beta Zeolite Catalysts — ***Michael Cordon**, Junyan Zhang, Nohor Samad, James W. Harris, Meijun Li, Dongxia Liu, Zhenglong Li*

4:54 Paper 679h: Direct Conversion of Renewable CO_2-Rich Syngas to High-Octane Hydrocarbons in a Single Reactor — ***Claire Nimlos**, Connor P. Nash, Dan Dupuis, Anh To, Jesse Hensley, Daniel Ruddy*

5:06 Paper 679i: Theoretical Study of the Direct Transformation of CO_2 and CH_4 into Surface CH_3coo Species on Single-Atom Alloys — ***Md Saeedur Rahman**, Ye Xu*

5:18 Paper 679j: Understanding Facet Dependent Selectivity Trends in Catalytic Hydrogenation and Hydrodeoxygenation of Lignin-Derived Aromatic Compounds — ***Haseena K V**, M. Ali Haider, Govind Porwal, C.P. Vinod*

5:30 Paper 679k: Kinetic Study of the Hydroxylation of Epoxidized Palm Oil Using NIR Spectroscopy for Reaction Monitoring — ***Wilson Felipe Bohorquez Malaver Sr.**, Alvaro Orjuela Sr., Jesus Garcia Sr., Steven Solarte Sr.*

(680) Resilient and Sustainable Supply Chains and Product Systems

Thursday, Nov 17, 3:30 PM
Phoenix Convention Center, N-226A

Simona Liguori, Chair
Vikas Khanna, Co-Chair
Ashley Pennington, Co-Chair

Sponsored by: Sustainability Science and Engineering

3:30 Paper 680a: Maximum Resiliency Identification for the General Refinery Supply Chain — *Li Yu, **Tianxing Cai**, Sujing Wang, Qiang Xu*

3:51 Paper 680b: Baseline Material Flow Systems Analysis of the PET and Polyolefin Plastics Supply Chains in the United States: Applications of MFA and LCA Data — ***Utkarsh Chaudhari**, Anne Johnson, Barbara Reck, Robert Handler, Vicki Thompson, Damon Hartley, Wendy Young, David W. Watkins, David Shonnard*

4:12 Paper 680c: Sustainable Waste Management Strategies and Technologies Moving Toward a Circular Economy — ***Tapas K. Das**, Murilo Innocentini, Heather Grob, Joseph M. Mailhot*

4:33 Paper 680d: Placement of Booster Chlorinator Based on Water Age Analysis for the Dead-End Sections of Drinking Water Distribution Network — ***Shanmugam V***

4:54 Paper 680e: Lithium Recovery from Unconventional Water Sources — ***Nathanial Cooper**, Boreum Lee, Sohum Patel, Ryan DuChanois, Menachem Elimelech*

5:15 Paper 680f: Screening and Ranking Eco-Innovations for Sustainable Circularity: Hotspot and Sensitivity-Based Optimization — ***Vyom Thakker**, Bhavik Bakshi*

(681) Sustainable Energy: Generation and Storage

Thursday, Nov 17, 3:30 PM
Phoenix Convention Center, N-226C

Vilas G. Pol, Chair
Sheila Samsatli, Co-Chair

Sponsored by: Sustainable Energy

3:30 Paper 681a: Flexible and Sub-Zero Temperature Functioning Porous Hydrogel Supercapacitor Modified By Chemical Crosslinking — ***Mina Shanbedi**, Alamgir Karim, Haleh Ardebili*

3:43 Paper 681b: Unveiling Flexibility of IrO_2 Crystal Structure: An Approach Towards Efficient Oer Catalysis — ***Waqas Qamar Zaman**, Waheed Miran*

3:56 Paper 681c: Characterizing Excess Energy Availability and Value — ***Micah Ziegler**, Aliza Khurram, Shannon Hwang, Jessika Trancik*

4:09 Paper 681d: Market-Integrated Optimization of Wind-Battery-Hydrogen Hybrids for Peaking Capacity Via Storage — ***Darice Guittet**, Bernard Knueven, Xian Gao, Jaffer Ghouse, Ignas Satkauskas, Alexander Dowling, Wesley Jones, John Siirola, David Miller*

4:22 Paper 681e: Generation and Storage of Green Hydrogen for the Decarbonisation of Energy-Intensive Industries: Whole-Systems Value Chain Optimisation — ***Sheila Samsatli**, Nouri John Samsatli*

4:35 Paper 681f: Dynamic Modeling and Control of Renewable Hydrogen Production, Storage and Consumption for Grid and Transportation Operations — ***Yifan Wang**, Sai Pushpitha Vudata, Paul Brooker, James Fenton*

4:48 Paper 681g: An Optimal Dispatch and Economic Performance Study of a Nuclear-Hydrogen Hybrid Energy System with Large-Scale Storage in Underground Salt Cavern — ***An Ho**, Daniel Hill, John Hedengren, Kody Powell*

5:01 Paper 681h: Improving Compressed Air Energy Storage Via Indirect Heat Transfer to a Thermochemical Reactor — ***Fuqiong Lei**, Eric Rebarchik, Alpha Toure, Nick AuYeung*

5:14 Paper 681i: Optimizing Absorption to Improve Haber-Bosch Synthesis — ***Chinomso Onuoha**, **Alon V. McCormick**, Cory Marquart, Matthew Palys, Zac Pursell, Ed Cussler, Prodromos Daoutidis, Michael Reese, Mahdi Malmali, Sameer Parvathikar, Deepak Ojha*

5:27 Paper 681j: Agile Ammonia Production through Process Integration for Medium to Long-Term Storage of Renewable Energy — ***Collin Smith**, Laura Torrente-Murciano*

5:40 Paper 681k: Optimal Allocation and Dispatch of Renewable Energy Systems Under Saudi Arabia's 2030 Vision and Climate Change Projections — ***Abdullah Maghfuri***

(682) CO2 Upgrading III: From Fundamental to Applied CO2 Electrocatalysis II

Friday, Nov 18, 8:00 AM
Phoenix Convention Center, N-128A

Ananth Govind Rajan, Chair
Anup Kumar Doraiswamy, Co-Chair

Sponsored by: Catalysis

8:00 Paper 682a: The Influence of Atomic-Scale Active Site Distributions on Selectivity in Electroreduction of CO_2 — ***Joakim Halldin Stenlid, PhD**, Joseph Gauthier, Martin Head-Gordon, Alexis T. Bell, Frank Abild-Pedersen*

8:18 Paper 682b: Electrochemical Conversion of Low Concentration CO2 Gas in a Membrane Electrode Assembly Electrolyzer — *Dongjin Kim, Ung Lee, Yun Jeong Hwang, **Dahye Won***

8:36 Paper 682c: Understanding the Dynamic Evolution of Atomically Dispersed Cu Catalyst for CO_2 Conversion to Ethanol Using Integrated in Situ and Computational Approach. — ***Jiayi Xu**, Prajay Patel, Di-jia Liu, Cong Liu*

8:54 Paper 682d: Laser-Made Copper-Free Nanocatalysts for Aqueous CO_2 Reduction to C–C-Coupled Products — ***Astrid Muller***

9:12 Paper 682e: Grain Boundary-Derived Cu^{+}/Cu^{0} Interfaces in CuO Nanosheets for Low Overpotential Carbon Dioxide Electroreduction to Ethylene — ***Zhengyuan Li***, *Jianfang Zhang, Jingjie Wu*

9:30 Paper 682f: Highly Productive and Selective CO_2-to-C_{2+} Conversion through *in-Situ* Spatial CO Management — ***Jingjie Wu***, *Tianyu Zhang*

9:48 Paper 682g: Mechanistic Insights Towards Selective C_3 Product Formation in $CO_{(2)}r$ on Copper — ***Michael Tang***, *Hongjie Peng, Joakim Halldin Stenlid, PhD, Frank Abild-Pedersen*

10:06 Paper 682h: Modeling Reactive Carbon Species in Bipolar Membranes for Carbon Capture and Conversion — ***Justin Bui***, *Alexis T. Bell, Adam Weber*

(683) Hydrocarbon Conversion I: Nonoxidative processes for hydrocarbon conversion

Friday, Nov 18, 8:00 AM
Phoenix Convention Center, N-127A

Melis Duyar, Chair
Thomas Senftle, Co-Chair
Apoorva Sridhar, Co-Chair

Sponsored by: Catalysis

8:00 Paper 683a: $[Pt_1\text{-}Zn_n]^{\delta+}$ Hybrid Cluster in HZSM-5 for Efficient Ethane Dehydroaromatization — ***Yizhi Xiang***, *Genwei Chen, Hossein Toghiani*

8:18 Paper 683b: Understanding the Speciation and Propane Dehydrogenation Activity in Zn/H-ZSM-5 Catalysts — ***Yong Yuan***, *Raul Lobo*

8:36 Paper 683c: Nonoxidation Coupling of Methane over Nano-Layer Platinum Catalysts on Two-Dimensional Metal Carbides (MXenes) — *Zhe Li,* ***Yang Xiao***, *Prabudhya Chowdhury, Zhenwei Wu, Tao Ma, Johnny Zhuchen, Gang Wan, Tae-Hoon Kim, Dapeng Jing, Peilei He, Pratik Potdar, Lin Zhou, Zhenhua Zeng, Xiulin Ruan, Jeffrey T. Miller, Jeffrey Greeley, Yue Wu, Arvind Varma*

3:30 Paper 683d: Overcoming Propane Dehydrogenation Equilibrium Limitations Using a Catalyst/Membrane Hollow Fiber System — ***Rawan Almallahi***, *James Wortman, Suljo Linic*

9:12: Break

9:30: Break

9:48 Paper 683g: Selectivity and Activity of Fe_3c As a Propane Dehydrogenation Catalyst — ***Peng Wang***, *Thomas Senftle*

10:06 Paper 683h: Influence of Carbonaceous Deposits on the Ferrierite Structure and Reactivity for the Skeletal 1-Butene Isomerization — ***Karoline Hebisch***, *Carsten Sievers*

(684) New Developments in Computational Catalysis: Efficiency and Automation

Friday, Nov 18, 8:00 AM
Phoenix Convention Center, N-127B

Matthew Montemore, Chair
Christopher Paolucci, Co-Chair

Sponsored by: Catalysis

8:00 Paper 684a: Towards Catalysis Informatics: How the Particularities of Catalytic Data Impact Machine Learning — *Pedro Mendes,* ***Florence Vermeire***, *Thibaut Van Haute, Joris Thybaut*

8:18 Paper 684b: Predicting the Morphology of Metal Nanoparticles Decorated with p-Block Promoters on-the-Fly — ***Asmee Prabhu***, *Tej Choksi*

8:36 Paper 684c: Machine Learning Screening of Alloy Surfaces for Catalytic Stability in Reaction Conditions — ***Gloria Sulley***, *Jihun Hamm, Matthew Montemore*

8:54 Paper 684d: Towards Swift Predictions of Metal Ad-Atom Diffusion Barriers and Surface Energies for Enhanced Understanding of Sintering and Catalysts Durability — ***Shyam Deo***, *Joakim Halldin Stenlid, PhD, Frank Abild-Pedersen*

9:12 Paper 684e: Developing a Theoretical Model to Unravel the Importance of Adsorbate Effects in Chemisorption on Surface Alloys — ***Shikha Saini***, *Joakim Halldin Stenlid, PhD, Frank Abild-Pedersen*

9:30 Paper 684f: Theory-Infused Neural Network for Interpretable Reactivity Prediction — ***Shih-Han Wang***, *Hemanth Pillai, Siwen Wang, Luke E. K. Achenie, Hongliang Xin*

9:48 Paper 684g: Open Challenges in Developing Generalizable Large Scale Machine Learning Models for Catalyst Discovery — ***Adeesh Kolluru***, *Muhammed Shuaibi, Aini Palizhati, Nima Shoghi, Abhishek Das, Brandon Wood, C. Lawrence Zitnick, John Kitchin, Zachary Ulissi*

10:06 Paper 684h: A Computational Workflow for Intermetallic Catalyst Discovery for Selective Hydrogenation Reactions — ***Angela Nguyen***, *Unnatti Sharma, Zachary Ulissi, Michael J. Janik*

(685) Nitrogen Chemistry: Thermal/photo/plasma N2 reduction

Friday, Nov 18, 8:00 AM
Phoenix Convention Center, N-127C

Meenesh Singh, Chair
Adam Nielander, Co-Chair

Sponsored by: Catalysis

8:00 Paper 685a: N_2 Activation and Spillover on Single-Atom Alloy Catalysts: A Theoretical Study — ***Chukwudi Nwaokorie***, *Gbolade Kayode, Matthew Montemore*

8:20 Paper 685b: Revisiting Ru As New Haber-Bosch Catalyst, Ru Nanoparticles Size and Shape Effect – Quantum Modelling — ***Luka Skubic***, *Sašo Gyergyek, Blaž Likozar, Matej Huš*

8:40 Paper 685c: Exploration of Novel Catalysts for Ammonia Synthesis: Creating a More Efficient Pathway — ***Samuel Drummond***, *Jennifer Naglic, Dr. Christopher T. Williams, Jochen Lauterbach*

9:00 Paper 685d: Engineered Bifunctional Alloys for Chemical Looping Ammonia Synthesis — ***Laron Burrows***, *George M. Bollas*

9:20 Paper 685e: Understanding the Influence of Photo-Thermal Inputs on Ammonia Synthesis Via Drifts — ***Carissa Yim***, *Alexander Hill, Andrej Lenert, Johannes Schwank*

9:40 Paper 685f: Low Temperature and Pressure Ammonia Synthesis Via Highly Dispersed Ruthenium Based Catalysts — ***Jennifer Naglic***, *Samuel Drummond, Abolfazl Shakouri, Dr. Christopher T. Williams, Jochen Lauterbach*

10:00 Paper 685g: N2 Cold DBD Plasma Activation and Low Pressure Large Scale NH3 Synthesis Process Design — ***Jonas Baltrusaitis***, *Guoqiang Cao, William L. Luyben, Robert Handler, Yue Xiao, Chien-Hua Chen*

(686) Reaction Engineering in Pharmaceuticals and Fine Chemicals

Friday, Nov 18, 8:00 AM
Phoenix Convention Center, N-128B

Luke Rogers, Chair
Gaurav Giri, Co-Chair

Sponsored by: Reaction Engineering

8:00 Paper 686a: Novel Green Chemistry Routes to High Purity Intermediates - Molecular Design and Process Intensification — ***Aaron Moment***, *Mengqi Shen, Hunter Vibbert, Ning Zhang*

8:18 Paper 686b: Slow Is Smooth and Smooth Is Fast: Implementation of Workflows for the Development of Processes and Equipment for the Manufacture of Critical Care Medicines — ***Gordon Brezicki***, *Tyler McQuade*

8:36 Paper 686c: Cyclodextrin Network Supported Catalysis in Flow — ***Bradley Davis***, *Jeffrey Bennett, Milad Abolhasani, Kirill Efimenko, Jan Genzer*

8:54 Paper 686d: Sustainable Sulfonated Carbon Catalysts for Continuous Esterification and Production of Biochemicals — ***Sarada Sripada***, *James Kastner*

9:12 Paper 686e: Realizing High Temperature Oxidations in Continuous Flow with Coupled Transport-Kinetic Modeling and Batch to Continuous Scale-up Experiments — ***Fatou Baka Diop***, *Ashli Silvera, Andrew R Teixeira*

9:30 Paper 686f: Diazomethane Permeability Study across Teflon AF 2400 Membrane Using Tube-in-Tube Module — ***Filip Horvath-Gerber***, *Klaus Hellgardt, Mimi Hii, Christian Holtze*

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(687) Software Engineering in and for the Molecular Sciences

Friday, Nov 18, 8:00 AM
Phoenix Convention Center, N-222B

Janani Sampath, Chair
Jacob Monroe, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

8:00 Paper 687a: VACUUMMS: stewardship of research software from the void — ***Frank Willmore***

8:22 Paper 687b: Polymerizeit! Software to Generate Molecular Structures of Crosslinked Polymers in silico — *Salman Bin Kashif,* ***Sapna Sarupria***

8:39 Paper 687c: Validating a New Force Field and Extensible Analysis for a Large-Scale Screening Study of P3HT — *Jenny Fothergill,* ***Eric Jankowski***

8:56 Paper 687d: MoSDeF-GOMC: Python software for the creation of scientific workflows for the Monte Carlo simulation engine GOMC — ***Brad Crawford***, *Umesh Timalsina, Co Quach, Nicholas C. Craven, Justin Gilmer, Peter Cummings, Jeffrey Potoff*

9:13: Break

9:21 Paper 687e: Chemprop: Machine Learning for Molecular Property Prediction — ***Charles McGill***, *Esther Heid, Yunsie Chung, Kevin Greenman, David Graff, Mengjie Liu, Camille Bilodeau, Rafael Gomez-Bombarelli, Connor Coley, Klavs Jensen, Tommi S. Jaakkola, Regina Barzilay, William Green*

9:38 Paper 687f: Workflow Automation in Predicting Exciplex Formation in Arene-Amine Complexes — ***Abhilash Patra***, *Shaama Mallikarjun Sharada*

9:55 Paper 687g: Parallelization of Grand Canonical Ensemble Monte Carlo Using Prefetching and Windowing of Flat Histogram Simulations — ***Harold Hatch***, *Vincent K. Shen*

10:12 Paper 687h: Pscf+: An Extended and Improved Open-Source Software Package for Polymer Self-Consistent Field Calculations of Block Copolymer Self-Assembly — ***Juntong He***, *Qiang Wang*

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(688) Applied Math for Biomedical Systems

Friday, Nov 18, 8:00 AM
Phoenix Convention Center, N-126C

Ashlee Ford Versypt, Chair
Mohammad Aminul Islam, Co-Chair

Sponsored by: Applied Mathematics and Numerical Analysis

8:00 Paper 688a: Predicting Therapeutic Efficacy on Renal Fibrosis in Diabetes: A Mathematical Model — ***Haryana Thomas***, *Ashlee Ford Versypt*

8:19 Paper 688b: Mathematical Modelling of Gene Delivery in Patients with Haemophilia B — ***Elnaz Jamili***, *Amit C. Nathwani, Vivek Dua*

8:38 Paper 688c: Compartmental Modeling of the Gastrointestinal (GI) Tract: Model Development and Validation in Predicting Gastric Emptying of Liquids — ***Shannon Fernandes***, *Mayuresh Kothare, Babak Mahmoudi, Charles Horn*

8:57 Paper 688d: Computational Fluid Particle Dynamics Illuminates Developmental Anatomical Feature Influence on Aerosol Deposition Patterns in 6-Year-Old Upper Airway CT-Scan Models — ***Emily Kolewe***, *Ian Woodward, Saurav Padhye, Jenna W. Briddell, Yu Feng, Catherine Fromen*

9:16 Paper 688e: Elimination of Noise and Sensor Drifts in Pediatric Pressure Transducers for the Prediction of Central Venous Catheter-Related Thrombosis Events — ***Daniel P. Howsmon***, *Katie Colman, Igor Arienamo, Matthew F. Mikulski, Richard P. Lion, Raajen Patel, Carlos M. Mery, Daniel Stromberg*

9:35 Paper 688f: A General Strategy for Optimal, Individualized Drug Dosing, Based on Hybrid Models and Dynamic Optimization Under Uncertainty — ***Francesco Rossi***, *Linas Mockus, Zoltan Nagy, Gintaras Reklaitis*

9:54 Paper 688g: Tipping Point Dynamics for Epidemiological Networks. Constructing Reduced Dynamical Data-Driven Models for Evolving Graphs — ***Nikolaos Evangelou***, *Tianqi Cui, Juan Bello-Rivas, Alexei Makeev, Thomas Bertalan, Ioannis G. Kevrekidis*

10:13 Paper 688h: Robustness of Machine Learning-Based Classifiers for Disease Diagnostics — ***Joshua Chuah***, *Ge Wang, Pingkun Yan, Juergen Hahn*

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(689) Modeling, Control and Optimization Applications

Friday, Nov 18, 8:00 AM
Phoenix Convention Center, N-126A

Maria Papathanasiou, Chair
Heleno Bispo, Co-Chair

Sponsored by: Systems and Process Control

8:00 Paper 689a: Integrated Design and NMPC-Based Control Under Uncertainty and Structural Decisions: A D-SDA and Mpcc-Based Strategy. — ***Oscar Palma-Flores***, *Luis Ricardez-Sandoval*

8:19 Paper 689b: A Systematic Safety-Oriented Process Design and Explicit Model Predictive Control Optimization Approach — ***Moustafa Ali***, *Xiaoqing Cai, Faisal Khan, Efstratios N. Pistikopoulos,* ***Yuhe Tian***

8:38 Paper 689c: Estimation-Based Model Predictive Control with State-Dependent Objective Prioritization; An Application to a Natural Gas Combined Cycle Power Plant — ***Daniel Beahr***, *Vivek Saini, Elijah Hedrick, Sung Min Choi Hong, Debangsu Bhattacharyya*

8:57 Paper 689d: Single and Multi-Objective Supervisory Model Predictive Control of Steam Temperature Cycles — ***Selorme Agbleze***, *Paolo Pezzini, Lawrence J. Shadle, Harry Bonilla-Alvarado, Rupendranath Panday, Natarianto Indrawan, David Tucker, Kenneth M. Bryden, Fernando V. Lima*

9:16 Paper 689e: Multivariable Run-to-Run Control of Thermal Atomic Layer Etching of Aluminum Oxide Thin Films — ***Sungil Yun***, *Matthew Tom, Feiyang Ou, Gerassimos Orkoulas, Panagiotis Christofides*

9:35 Paper 689f: Modeling of Anaerobic Digester Using Anaerobic Digestion Model No. 1 (ADM1) in Idaes/Pyomo — ***Mayowa F. Oladele***, *George M. Bollas*

9:54 Paper 689g: Experimental Design for Estimating "Just-in-Time" States in Control-Oriented Behavioral Interventions for Physical Activity — ***Mohamed El Mistiri***, *Daniel Rivera, Junghwan Park, Meelim Kim, Predrag Klasnja, Eric Hekler*

10:13 Paper 689h: Application of Gaussian Processes to Online Approximation of Compressor Maps for Load-Sharing Optimization — ***Akhil Ahmed***, *Marta Zagorowska, Antonio del Rio Chanona, Mehmet Mercangoez*

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(690) Operation of Energy Systems

Friday, Nov 18, 8:00 AM
Phoenix Convention Center, N-126B

Mariano Martin, Chair
Q. Peter He, Co-Chair

Sponsored by: Systems and Process Operations

8:00 Paper 690a: Remuneration of Energy Storage in Electricity Markets Using Virtual Links — ***Weiqi Zhang***, *Victor Zavala*

8:18 Paper 690b: Data-Driven Modeling and Optimization of Bidirectional Electric Vehicle Dispatch in Low-Carbon Power Systems — ***James Owens***, *Ian Miller, Emre Gençer*

8:36 Paper 690c: Globally Optimal Design and Operation of an Air-Cooled Geothermal Organic Rankine Cycle — *Marco Langiu, Manuel Dahmen,* ***Alexander Mitsos***

8:54 Paper 690d: Power Distribution Networks with Mobile Green Ammonia-Fueled Power Generation — ***Benjamin Riley***, *Prodromos Daoutidis, Qi Zhang*

9:12 Paper 690e: Modeling and Optimization of Mixed Hydrogen-Natural Gas Flow in Pipeline Network — ***Saif Kazi***, *Kaarthik Sundar, Anatoly Zlotnik, Shriram Srinivasan*

9:30 Paper 690f: Optimization Opportunities for Stand-Alone Liquid Air Energy Storage — *Zhongxuan Liu,* ***Truls Gundersen***

9:48 Paper 690g: Multi-Objective Dynamic Optimization of Natural Gas Combined Cycle (NGCC) Plant Load-Following Operation with Equipment Health Constraints — ***Yifan Wang***, *Debangsu Bhattacharyya*

10:06 Paper 690h: Open-Source Capacity Expansion Model with a Focus on Accessibility, Usability, and Complete Life-Cycle Assessment — ***Amanda Farnsworth***, *Ian Miller, Emre Gençer*

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(691) Modeling of Lipid Membranes and Membrane Proteins

Friday, Nov 18, 8:00 AM
Phoenix Convention Center, N-222C

Diwakar Shukla, Chair
Reid Van Lehn, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

8:00 Paper 691a: Exploring the Mechanism of Mutation Induced Surfactant Protein D's Higher Antiviral Activity at the Molecular Level — ***Mona Minkara***

8:15 Paper 691b: Molecular Simulations of Activating and Inhibitory Protein Interactions in Triglyceride-Rich Lipoprotein Metabolism — ***Emma Lietzke***, *Kimberley Bruce, Kayla Sprenger*

8:30 Paper 691c: Developing Hyper-Elastic Liposomes for Enhanced Drug Delivery: Insights from Molecular Simulations — ***Jiaming Xu***, *Vyshnavi Karra, Danielle Large, Debra Auguste, Francisco Hung*

8:45 Paper 691d: Modeling Complex Lipid Bilayers to Investigate the Diffusion of Antiretroviral Drugs across the Blood-Brain Barrier — ***Daisy Fuchs***, *Kayla Sprenger*

9:00 Paper 691e: Multiscale Modeling of Stratum Corneum Lipids — ***Chloe Frame***, *Parashara Shamaprasad, Christopher Iacovella, Annette Bunge, Clare McCabe*

9:15 Paper 691f: Molecular Mechanisms of Helix Flipping across Lipid Bilayers — ***Reid Van Lehn***

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(692) Design and Optimization of Integrated Energy Systems II

Friday, Nov 18, 8:00 AM
Phoenix Convention Center, N-225B

Alexander Dowling, Chair
Dhabia Al-Mohannadi, Co-Chair
David Miller, Co-Chair

Sponsored by: Climate Change

8:00 Paper 692a: Multiperiod Design Optimization of a Flexible Power-to-Methanol Process — ***Andrea Maggi***, *Jens Bremer, Kai Sundmacher*

8:21 Paper 692b: Dynamic Modeling and Simulation of a Novel Nuclear-Hydrogen Hybrid Energy System with Large-Scale Storage in an Underground Salt Cavern. — ***An Ho***, *Kasra Mohammadi, Matthew Memmott, John Hedengren, Kody Powell*

8:42 Paper 692c: Technoeconomic Analysis and Optimization of Low Carbon, Reforming-Based Integrated Energy Systems for the Co-Production of Hydrogen and Power — ***Maojian Wang***, *Jinliang Ma, Eric Lewis, Paul Myles, John Brewer, Dale Keairns, Anthony P. Burgard, David Miller*

9:03 Paper 692d: Analysis and Validation of an Electrified Steam-Methane Reforming Process — *Cornelius Masuku,* ***Yufei Zhao***

9:24 Paper 692e: Conceptual Design and Analysis of a Power Generator with Integrated Thermal Energy Storage and CO_2 Capture — ***Naresh Susarla***, *Edna Rawlings, Jaffer Ghouse, John Siirola, David Miller*

9:45 Paper 692f: Integrated Design and Operation of Low-Carbon District Heating Systems — ***Gustavo Campos***, *Nael El-Farra, Ahmet Palazoglu*

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(693) Cell-free systems and DNA assembly platforms

Friday, Nov 18, 8:00 AM
Phoenix Convention Center, N-125B

Yanran Li, Chair
Gozde Demirer, Co-Chair

Sponsored by: Bioengineering

8:00: Break

8:18 Paper 693b: Engineering Transmembrane Signal Transduction in Synthetic Vesicles Using Two Component Systems — ***Justin Peruzzi***, *Neha Kamat*

8:36 Paper 693c: Plasmidmaker: A Versatile, Automated, and High Throughput End-to-End Platform for Plasmid Construction — ***Behnam Enghiad***, *Pu Xue, Nilmani Singh, Aashutosh Boob, Chengyou Shi, Vassily Andrew Petrov, Roy Liu, Siddhartha Suryanarayana Peri, Stephan Thomas Lane, Huimin Zhao*

8:54 Paper 693d: Development and Assembly of a Synthetic Membrane-Less Enzymatic ATP Regeneration Cascade Powered By Fuel Oxidation — *Scott Banta,* ***Emma Willett***

9:12 Paper 693e: Using the Cell-Free Gene Expression System for Highly Accurate Microrna Detection — ***Caroline Copeland***, *Yongchan Kwon*

9:30 Paper 693f: Profiling of Putative Threonine Transaldolases for Biosynthesis of Non-Standard Amino Acids — ***Michaela Jones***, *Neil Butler, Sean Wirt, Ishika Govil, Shelby Anderson, D'Jana Wyllis, Aditya Kunjapur*

9:48 Paper 693g: Enabling Exquisite Control in Cell-Free Biomanufacturing with Orthogonal Redox Cofactors — ***Han Li***

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(694) Systems and Quantitative Biology: Disease Mechanisms and Therapies

Friday, Nov 18, 8:00 AM
Phoenix Convention Center, N-125A

Kate Galloway, Chair
Junyoung Park, Co-Chair

Sponsored by: Bioengineering

8:00 Paper 694a: Mathematical Modeling of Dysregulation of ACE2 Depending on Age-Sex and Blood Pressure and Progression of Fibrosis in COVID19 Survivors — ***Mohammad Aminul Islam***, *Ashlee Ford Versypt*

8:18 Paper 694b: Cell-Free RNA Liquid Biopsies at Cell Type Resolution in Health and Disease — ***Sevahn Vorperian***, *Mira Moufarrej, Stephen Quake*

8:36 Paper 694c: Coupled Quantitative Transcriptomic and High-Throughput Morphological Analysis Predict Biological Effects of Environmental Toxins on Human Lung Cells — ***Sean Engels***, *Pratik Kamat, Daniel Haller, Jude Phillip, Lydia Contreras*

8:54 Paper 694d: A Logic-Based Modeling Study of Glucose Mediated Immune Response in Diabetic Kidney Disease — ***Krutika Patidar***

9:12: Break

9:30 Paper 694f: Temporal Analysis of Autophagy Rates and Subcellular Morphological Dynamics Using High-Throughput Image-Based Single Cell Profiling — *Nitin Sai Beesabathuni, Soyoon Park, Eshan Thilakaratne,* ***Priya Shah***

9:48 Paper 694g: Integrative Approaches to Elucidate Mechanisms of Neurological Disorders — ***Tamara L. Kinzer-Ursem***

(695) Process Intensification in Biorefineries

Friday, Nov 18, 8:00 AM
Phoenix Convention Center, N-228A

Sridharan Ramaswamy, Chair
Yaseen Elkasabi, Co-Chair

Sponsored by: Forest and Plant Bioproducts Division

8:00 Paper 695a: Simultaneous Biomass Fractionation and Xylan Conversion Using Deep Eutectic Solvents — *Caixia Wan,* ***Qianwei Li***

8:15 Paper 695b: Reinforced Learning Based Control Algorithm for Anarobic Digestion Under Feedstock Uncertaint — ***Abigael Wahlen****, Ji Gao, Caleb Ju, Guanghui Lan, Zhaohui Tong*

8:30 Paper 695c: Renewable Tar Pitch Based on Pyrolysis Bio-Oils. — ***Yaseen Elkasabi****, Charles A. Mullen*

8:45 Paper 695d: Green Synthesis of Agnp-Based Potent Antimicrobial Agents Using Lignin-Containing Nanocelluloses — ***Caixia Wan****, Yisheng Sun*

9:00 Paper 695e: Experimental Analysis of Convective Drying of Paper and Board — *Koushik Sampath, Leonard Reynolds, Michael Ringold, Xinyi Li, Huajiang Huang,* ***Sridharan Ramaswamy***

9:15 Paper 695f: Process Evaluation of Lignocellulosic Resource Treatment for Sustainable Corrosion Inhibitor of Carbon Steel — ***Tianxing Cai***

(696) Accelerated Discovery of Inorganic Materials: High-Throughput Experiments, Modeling, and Data Science

Friday, Nov 18, 8:00 AM
Phoenix Convention Center, N-122A

Peng Bai, Chair
Camille Bilodeau, Co-Chair
Satish Nune, Co-Chair

Sponsored by: Inorganic Materials

8:00: Break

8:18 Paper 696b: A DFT Analysis of Optimal Solvents for High-Throughput Processing of Imine-Linked Cofs — ***Obioma Uche****, Emily Rankin*

8:36 Paper 696c: Influence of Missing Linker and Missing Cluster Defects on the Thermal Conductivity of Metal-Organic Framework UiO-66 — ***Meiirbek Islamov****, Christopher E. Wilmer*

8:54 Paper 696d: High-Throughput DFT Dataset of Theoretical Multinary Perovskite Oxides — *Zachary Bare,* ***Ryan Morelock****, Charles B. Musgrave*

9:12 Paper 696e: Thermodynamic Stability and Anion Ordering in ABO_2n and $ABON_2$ Perovskite Oxynitrides — ***Sam Young****, Bianca Ceballos, Amitava Banerjee, Ghanshyam Pilania, Bryan Goldsmith*

9:30 Paper 696f: A Computational Framework to Accelerate the Discovery of Perovskites for Solar Thermochemical Hydrogen Production; Identification of Gd Perovskite Oxide Redox Mediators — ***Zachary Bare****, Ryan Morelock, Charles B. Musgrave*

9:48 Paper 696g: Autonomous Synthesis of Metal Halide Perovskite Nanocrystals — ***Fazel Bateni****, Robert Epps, Kameel Abdel-Latif, Rokas Dargis, Jeffrey Bennett, Kristofer G. Reyes, Milad Abolhasani*

10:06 Paper 696h: Development of a High-Throughput Workflow for the Synthesis of CdSe Nanocrystals Using a Sonochemical Materials Acceleration Platform — ***Maria Politi****, Fabio Baum, Kiran Vaddi, Brittany Bishop, Joshua Vasquez, Vincent Holmberg, Nadya Peek, Lilo Pozzo*

(697) Data-Driven/Machine Learning-Enabled Design for Nanocomposites

Friday, Nov 18, 8:00 AM
Phoenix Convention Center, N-121B

Po-Yen Chen, Chair
Sandra Ike, Co-Chair
Amanda Koh, Co-Chair

Sponsored by: Composites

8:00 Paper 697a: Machine Learning–Enabled Design of All-Natural Plastic Substitutes — ***Tianle Chen****, Shuaiming He, Haitao Yang, Snehi Shrestha, Joshua Little, Po-Yen Chen*

8:20 Paper 697b: Accelerated Design of Flame Retardant Polymeric Nanocomposites Via Machine Learning — ***Zhuoran Zhang****, Zeren Jiao, Ruiqing Shen, Qingsheng Wang*

8:40 Paper 697c: Machine Learning Assisted Development of Electrochemical Cortisol Sensor Based on Electropolymerized Molecularly Imprinted Polymer — *Grace Dykstra, Kai Zhou,* ***Yixin Liu***

9:00 Paper 697d: Data-Driven Design of Mxene Aerogels with Programmable Mechanical Performance Via Active Learning and Collaborative Robots — ***Snehi Shrestha****, Po-Yen Chen, Tianle Chen, Shuaiming He*

9:20 Paper 697e: Monitoring Catalysts Synthesis Using Real-Time Emission Spectroscopy and Advanced Machine Learning Models — ***Can Wang****, Ben Ko, Musa Najimu, Erdem Sasmaz*

9:40 Paper 697f: Automatic Stretchable Conductor Design and Fabrication Via Machine Learning — ***Haochen Yang****, Po-Yen Chen*

(698) Fundamental Theory and Characterizations for Optoelectronic Materials

Friday, Nov 18, 8:00 AM
Phoenix Convention Center, N-121C

Charles Hages, Chair
Brett Savoie, Co-Chair

Sponsored by: Electronics and Photonics

8:00 Paper 698a: Computational Search for Halide Double Perovskite Optoelectronics — ***Christopher J. Bartel***

8:30 Paper 698b: Seeing Single Atoms in Materials Via Atomic Electron Tomography — ***Saman Moniri****, Yao Yang, Yakun Yuan, Jihan Zhou, Xuezeng Tian, Dennis S. Kim, Dillan J. Chang, Minh Pham, Colum M. O'Leary, Fan Zhu, NaYeon Kim, Yonggang Yao, Christopher J. Ciccarino, Yasutaka Nagaoka, Ou Chen, Prineha Narang, Andreas K. Schmid, Colin Ophus, Hao Zeng, Hendrik Heinz, Liangbing Hu, Peter Ercius, Jianwei Miao*

8:42 Paper 698c: Mechanistic Insights into Plasmonic Photocatalysis By Dynamic Calculations — ***Connor Herring****, Matthew Montemore*

8:54 Paper 698d: First Principles Approach to Understanding Stability in Ge-Sn Nanomaterials — *Katelyn P. Nelson, Mattea K. Miller, Deep Patel,* ***Luke Roling***

9:06 Paper 698e: Enhanced Bayesian Parameter Estimation from Time-Resolved Photoluminescence Data through an Adaptive Metropolis Sampler — ***Calvin Fai****, Anthony J. C. Ladd, Charles Hages*

9:18 Paper 698f: Self-Assembly of Donor-Acceptor Conjugated Polymer in the Condensed Phase — ***Chinmoy Saha****, Md Masrul Huda, Neeraj Rai*

9:30 Paper 698g: Pit Rim Decomposition into Multiple Quantum Dots on Surfaces of Epitaxial Thin Films Grown on Pit-Patterned Substrates — ***Omeet Patel****, Chao-Shou Chen, Dimitrios Maroudas*

9:42 Paper 698h: Stimuli-Responsive Stabilized Blue Phase Liquid Crystals Microdroplets — ***Sepideh Norouzi***, *Monirosadat Sadati*

9:54 Paper 698i: Materials Behavior at Electrochemical Interfaces: Insights from Theory and Computation — ***Perla Balbuena***

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(699) Transport Phenomena in Polymer Systems

Friday, Nov 18, 8:00 AM
Phoenix Convention Center, N-122B

Ryan Poling Skutvik, Chair
Steve R. Lustig, Co-Chair
Maninderjeet Singh, Co-Chair

Sponsored by: Polymers

8:00 Paper 699a: Electrophoretic Transport through Fibrocartilage Driven By Pulsed and Sawtooth Waveforms with Decreased Joule Heating. — ***Prince Atsu***

8:15 Paper 699b: 3D Printed Polymer Adsorbers for Capturing Chemotherapy Drugs before They Spread through the Body — ***Hee Jeung Oh***

8:45 Paper 699c: Modeling Water Imbibition of Hydrogel Coated Seeds — ***Tori Phillips***, *Jean-Francois Louf*

9:00 Paper 699d: High Throughput Platform for Macromolecular Transport — ***Paulina Babiak***, *Mazin Hakim, Adib Ahmadzadegan, Qinghua Xu, Pavlos Vlachos, Luis Solorio, Julie C. Liu*

9:15: Break

9:30 Paper 699f: Effect of Chain-End Group in Higly Polar Yet Amorphous Poly(1,3-dioxolane)-Based Polymers on Gas Separation Properties — ***Thien Tran***, *Liang Huang, Shweta Singh, Haiqing Lin*

9:45 Paper 699g: Dissolution of Semicrystalline Polyethylene — *Ali Ghasemi, Christian Ferger, Paschalis Alexandridis,* ***Marina Tsianou***

10:00 Paper 699h: Diffusion of CO_2 in an Amine-Cured Epoxy Novolac Coating at HPHT Conditions: Cause of Underfilm Corrosion — ***Narayanan Rajagopalan***, *Claus Erik Weinell, Kim Dam-Johansen, Søren Kiil*

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(700) Advancements in Particle Engineering and Material Sciences in Pharmaceutical Process Development II

Friday, Nov 18, 8:00 AM
Phoenix Convention Center, N-123

Parind Desai, Chair
Srivatsan Ramesh, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

8:00 Paper 700a: Two-Dimensional Population Balance Model for Twin-Screw Wet Granulation: Model Development and Calibration Based on Particle Size Distribution and Porosity — ***Kensaku Matsunami***, *Ana Alejandra Barrera Jimenez, Michiel Peeters, Michael Ghijs, Daan Van Hauwermeiren, Thomas De Beer, Ingmar Nopens*

8:21 Paper 700b: Machine Learning Approaches for the Prediction of Powder Behavior of Pharmaceutical Formulations from Physical Properties of the Active Pharmaceutical Ingredient — ***Laura Pereira Diaz***, *Stephanie Marchal, Patrick M. Piccione, Cameron Brown, Alastair J. Florence*

8:42 Paper 700c: Impact of Material Attributes on Continuous Mixing Quality: A DEM Study — ***Peter Toson***, *Marko Matic, Johan Remmelgas, Dalibor Jajcevic, Jakob Rehrl, Michela Beretta, Thomas O'Connor, Abdollah Koolivand, Geng Tian, Scott M. Krull, Johannes G. Khinast*

9:03 Paper 700d: *Agglomeration of Fine APIs As a Material Sparing Screening Indicator for Powder Processability* — ***Sangah Kim***, *Mirna Cheikhali, Rajesh Dave*

9:24 Paper 700e: Engineering of Spherical Lactose and D-Mannitol: Improving Excipient Particles for the Optimized Manufacture of Pharmaceutical Solid Dosage Forms — ***Joana Pinto***, *Sarah Zellnitz-Neugebauer, Christina Winter, Amrit Paudel*

9:45 Paper 700f: Developing a Roadmap to Effectively Spray Dry Biomolecules. — ***Laura Foley***, *Ahmad Ziaee, Alice Parkes, Emmet O'Reilly*

10:06 Paper 700g: Lipid-Based Particle Engineering Via Spray-Drying for Drug Targeting to the Lung — *Đana Crvenjak,* ***Carolina Corzo***, *Sharareh Salar-Behzadi, Sebastian Reyer, Dirk Lochmann, Andreas Zimmer*

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(701) Computational approaches to DoE and better process understanding

Friday, Nov 18, 8:00 AM
Phoenix Convention Center, N-122C

Yuriy Abramov, Chair
Ebenezer Ojo, Co-Chair
Daniel Hallow, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

8:00 Paper 701a: Application of Hybrid Modeling Approaches Towards Accelerated Process Characterization — ***Andrew Fiordalis***, *Jackie Gonzalez, Karthik Boppidi, Michael Skoumal, Tolutola Oyetunde*

8:25 Paper 701b: Risk Mitigation in Model-Based Experiment Design: A Continuous-Effort Approach to Optimal Campaigns — ***Kennedy Kusumo***, *Kamal Kuriyan, Shankar Vaidyaraman, Salvador Garcia Munoz, Nilay Shah, Benoit Chachuat*

8:50 Paper 701d: Application of a Mechanistic Model for Ultrafiltration and Diafiltration for Process Troubleshooting and Design Space Exploration — ***Maxwell Maritato***, *Harun Ozbakir, Xiaoxiang Zhu, Dongying Shen, Joseph Pollastrini, Pablo A. Rolandi*

9:15 Paper 701e: Automated Multi-Task Bayesian Optimization of Pharmaceutical Processes — ***Connor Taylor***

9:40 Paper 701f: Hybrid-Modeling Approaches for Rapid Quantification of Reaction Kinetics — ***Boung Wook Lee***, ***Anastasia Nikolakopoulou***, *Mikael Arnold, Xiao Li*

10:05 Paper 701g: A Fit for Purpose Kinetic Model to Understand the Knowledge Space of a Complex Telescopic Reaction Scheme — ***Maitraye Sen***, *Alonso J. Arguelles*

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(702) Antifouling Membranes for Water Purification

Friday, Nov 18, 8:00 AM
Phoenix Convention Center, N-131C

Steven Weinman, Chair

Sponsored by: Membrane-Based Separations

8:00 Paper 373j: Implications of Shear and Cation Choice on Dynamics of Nonliving Natural Organic Matter — ***Kathlyn Mealio***, *Holly A. Stretz, Martha J. M. Wells, Katherine Slamen, John Clark*

8:21 Paper 702b: Study of MF Membranes for Microalgae Dewatering and Surface Modification for Fouling Mitigation — ***Erda Deng***, *Xiaoyi Chen, Darius Rub, Haiqing Lin*

8:42 Paper 702c: Functionalized Magnetic Metal Organic Framework Thin-Film Nanocomposite Membranes with Real-Time Induced Vibrations for Enhanced Antifouling — ***Jasneet Pala***, *Ryan Tracy, Nima Mahmoodi, Milad Esfahani*

9:03 Paper 702d: Development of a Modular Shipboard Wastewater Reuse System — *Nathaniel Michael,* ***Andrew Wagner***

9:24 Paper 702e: Combined QCM-D/MP-SPR for Early-Stage Membrane Fouling Detection with Unprecedented Senstivity — ***Thomas Schafer***, *Iliane Rafaniello*

9:45 Paper 702f: Towards Understanding Cake Formation and Filtration Characteristics for Enhanced Media Filtration in Effluent Waste Management — ***Mutiu Amosa***, *Gbenga Komolafe, Olatokunbo S. Karimu, Mohammed Saedi Jami, Fatai Alade Aderibigbe, Adewale George Adeniyi, Tamrin Bin Tajari, Bisola Taibat Bello*

10:06 Paper 702g: IMAGE Processing As a Tool in Fouling Characterization for Reverse Osmosis Desalination — ***Tu Pham Le Phuong***, *Jisha Ali, Mohamed Soufiane Jouini, Emad Alhseinat*

(703) CO_2 Capture By Adsorption

Friday, Nov 18, 8:00 AM
Phoenix Convention Center, N-130

Youssef Belmabkhout, Chair
Stefano Brandani, Co-Chair

Sponsored by: Adsorption and Ion Exchange

8:00 Paper 703a: Development of Sodium-Borate Adsorbent for CO_2 capture at High Temperature from Flue Gas Stream — *Turki Alghamdi, Qasim Al-Naddaf, Fateme Rezaei,* ***Ahmed Al-mamoori***

8:16 Paper 703b: New Adsorbent for Post-Combustion CO_2 Capture: Modification of 13X Zeolite By Molecular Layer Deposition — ***James A. Ritter***, *Armin Ebner, Huan Jiang, Charles E. Holland, Ryan Sanders, Richard Ciora, Dong Qiaobei, Brian Sengupta, Miao Yu*

8:32 Paper 703c: Direct Air Capture (DAC) of CO_2 Using a Tailored Chelating Exchanger at Ambient Temperature — ***Arup SenGupta***

8:48 Paper 703d: Entrapment of Small Amines in Mesoporous Silica Via Polymeric Coating for the Direct Air Capture of CO_2 — ***Kaleb Friedman***, *Shailesh Dangwal, Miao Yu*

9:04 Paper 703e: Amine-Impregnated Al_2O_3 Materials for the Direct Air Capture of CO_2 Under Sub-Ambient Conditions — ***Pranjali Priyadarshini***, *Guanhe Rim, Cornelia Rosu, Mingyu Song, Fanhe Kong, Ryan P. Lively, Christopher W. Jones*

9:20 Paper 703f: Improving the Hydrothermal Stability of Amine-Grafted MCM-41 Silica Via Incorporation of Aluminum into the Structure of the Support — ***Masoud Jahandar Lashaki***, *Hessam Ziaei, Abdelhamid Sayari*

9:36 Paper 703g: Study of Carbon Mineralization at the Surface of Mg- and Ca-Based Oxides — ***Colin Lehman-Chong***, *Ella M. Siefken, Aleksandra Vojvodic*

9:52 Paper 703h: Moisture-Controlled CO_2 Capture and Electrochemical CO_2 Capture — ***Yuta Kaneko***, *Matthew D. Green, Klaus S. Lackner*

10:08 Paper 703i: Process-Based Screening of MOFs for Direct Air Capture (DAC) — ***Bhubesh Murugappan Balasubramaniam***, *Ohmin Kwon, Jun Luo, Marco Gibaldi, Tom Woo, Phuc-Tien Thierry, Samuel Lethier, Philip Llewellyn, Cecile Pereira, Veronique Pugnet, Arvind Rajendran*

(704) Diffusion, Transport and Dynamics in Adsorption Systems

Friday, Nov 18, 8:00 AM
Phoenix Convention Center, N-131B

Aaron Moran, Chair
Yu Wang, Co-Chair

Sponsored by: Adsorption and Ion Exchange

8:00 Paper 704a: Polyethylene in Dead End Silica Nanopores: Forces and Mobility from Non-Equilibrium Statistical Mechanics and Exsy NMR — ***Ziqiu Chen***, *Baron Peters, Frédéric Perras*

8:20 Paper 704b: Analysis of the Non-Isothermal Model for Volumetric Diffusion Measurements — ***Stefano Brandani***, *JinYu Wang, Enzo Mangano, Federico Brandani, Pluton Pullumbi*

8:40 Paper 704c: The Synthesis of Hierarchical SAPO-34 Zeolite and Potential Adsorption Applications — *Obaid Khan, Ninad D. Anjikar, Orhan Talu,* ***Shaowei Yang***

9:00 Paper 704d: Effect of Particle of Size on the Single Gas Diffusion of CO_2 and N_2 in 13X Zeolite Using a 100 Hz Volumetric Frequency Response System — ***Armin Ebner***, *Sarah Gustafson, Adam M. Burke, Charles E. Holland, James A. Ritter*

9:20 Paper 704e: Unraveling Water-Ion Dynamics in Reverse Osmosis Membranes with Nuclear Magnetic Resonance Spectroscopy — *Marta Hatzell,* ***Mahsa Abbaszadeh***

9:40 Paper 704f: Investigation of CO_2 Adsorbents for Direct Air Capture: Equilibrium, Kinetic, and Stability Data — ***May-Yin Low***, *David Danaci, Hassan Azzan, Lucy Victoria Barton, Camille Petit*

10:00 Paper 704g: Iron-Based Metal-Organic Framework for Superfast Adsorption of Uncharged Urea from Water: Synthesis, Characterization and Mechanism — ***Tin Le***, *Milad Esfahani*

(705) Mixed-Matrix Materials for Gas Separation

Friday, Nov 18, 8:00 AM
Phoenix Convention Center, N-132A

Michele Galizia, Chair
Zachary Smith, Co-Chair

Sponsored by: Membrane-Based Separations

8:00 Paper 705a: Synthesis and Characterization of NOVEL MIXED Matrix Membrane Comprises of Bimetallic Metal Organic Framework for Separation of Carbon Dioxide from Methane — ***Zartasha Azhar***

8:20: Break

8:41 Paper 705c: Facile Defect Engineering of Zeolitic Imidazolate Frameworks Towards Enhanced Propylene/Propane Separation Performance — ***Heseong An***, *Jong Suk Lee*

9:01 Paper 705d: Facile Approach to Simultaneously Reducing Physical Aging and Swelling While Enhancing Permeability in Microporous Polymer Membranes — *Jing Deng, Cara M. Doherty, William Box, Laura Matesanz Niño, Angel Lozano, Cristina Álvarez, Anita J. Hill,* ***Michele Galizia***

9:21 Paper 705e: One-Step Fabrication of Highly Propylene-Selective Asymmetric Mixed-Matrix Membranes with *in-Situ* ZIF-8 Filler Formation — ***Yinying Hua***, *Sunghwan Park, Hae-Kwon Jeong*

9:41 Paper 705f: Tailoring Ultramicropores in Hybrid Carbon Molecular Sieve Membranes to Achieve High H_2 Selectivity — ***Leiqing Hu***, *Vinh Bui, Ashwanth Subramanian, Kim Kisslinger, Lingxiang Zhu, Shouhong Fan, Yifu Ding, Chang-Yong Nam, Haiqing Lin*

10:01 Paper 705g: Tunable Supramolecular Cavities Molecularly Homogenized in Polymer Membranes for Ultraefficient Precombustion CO_2 Capture — ***Ji Wu***, *Can-Zeng Liang, Ali Naderi, Tai-Shung Chung*

10:21 Paper 705b: Thin Film Composite/Nanocomposite Membranes for Helium Recovery and Purification — *Cansu Yildirim, Melis Tok Şimşek,* ***Serife Birgül Tantekin-Ersolmaz***

(706) Structured Adsorbents: Beyond Pellets and Beads

Friday, Nov 18, 8:00 AM
Phoenix Convention Center, N-131A

Joeri Denayer, Chair
Fateme Rezaei, Co-Chair

Sponsored by: Adsorption and Ion Exchange

8:00 Paper 706a: 3D Printed Hybrid Monolith for CO2 Capture — ***Ana Pereira***, *Alexandre Ferreira, Alírio E. Rodrigues, Ana M. Ribeiro, Maria João Regufe*

8:20 Paper 706b: Development of an Expanded PTFE Structured Adsorbent Containing Activated Carbon — ***Sulaimon Adegunju***, *Ryan Sanders, Behnam F. Kisomi, Charles E. Holland, Armin Ebner, Guo Shiou Foo, Bob Grasso, Steve K. Stark, Jeff Knopf, Joe W. Henderson, James A. Ritter*

8:40 Paper 706c: Membrane Adsorbents Comprising Self-Assembled Inorganic Nanocages (SINCs) for Direct Air Capture — ***Thien Tran***, *Shweta Singh, Amanda Grass, Timothy R. Cook, Haiqing Lin*

9:00 Paper 706d: Sub-Ambient Direct Air Capture of CO_2 Using MIL-101(Cr) Monoliths — ***Yuxiang Wang***, *Guanhe Rim, Mingyu Song, Christopher W. Jones, Ryan P. Lively*

9:20 Paper 706e: Modelling and Experimentation on a Rotary Adsorber Applied to Direct Air Capture — ***Lucy Victoria Barton***, *Camille Petit, Ronny Pini*

9:40 Paper 706f: Immobilization of Zeolite Crystals on Coc-Based Microfluidic Devices for Separation Processes — ***Fadi Dawaymeh***, *Nahla Alamoodi, Anas Alazzam, Maryam Khaleel*

10:00 Paper 706g: Encapsulating Nanoscale Organic Hybrid Materials (NOHMs) within Polymeric Nanofibers Via Electrospinning for CO2 Capture — ***Jeffrey Xu***, *Ga Hyun Lee, Kyle Kersey, Dongjae Kim, Michelle Kidder, Yong Joo, Ah-Hyung Alissa Park*

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(707) CO2 Upgrading IV: Photo/Reduction, Hydrogenation, and Dual Capture/Conversion Systems

Friday, Nov 18, 12:30 PM
Phoenix Convention Center, N-128A

Melis Duyar, Chair
Astrid M. Mueller, Co-Chair

Sponsored by: Catalysis

12:30 Paper 707a: Direct and Continuous Generation of Pure Liquid Fuels Via Electrocatalytic Carbon Dioxide Reduction — ***Peng Zhu***

12:48 Paper 707b: Mie Resonance Induced Photocatalytic CO_2 Reduction Using Earth Abundant Dielectric Nanostructures — ***Sundaram Bhardwaj Ramakrishnan***, *Ravi Teja Addanki Tirumala, Marimuthu Andiappan*

1:06 Paper 707c: Highly Ordered Copper Nanowire Array As Active Electrocatalysts for CO_2 Reduction Reaction — ***Zhengyang Yang***, *Fanglin Che, Zhiyong Gu*

1:24 Paper 707d: Exsolution of Nife Nanoparticles on Ni-Doped (La,Sr)FeO_3: Its Effect on Co-Electrolysis of CO_2 and H_2o for Syngas Production — ***Jaesung Kim***, *Matthew Ferree, Seval Gunduz, Dhruba Jyoti Deka, Jean-Marc Millet, Anne Co, Umit Ozkan*

1:42 Paper 707e: Ligand-Assisted Electrodeposition of Copper Catalyst: Towards Electrochemical Carbon Dioxide Reduction to Multi-Carbon Products — ***Lei Wang***

2:00 Paper 707f: Optimizing Operating Conditions for Solar Driven CO_2 Reduction Using High Performance GaAs and Silicon-Based Photocathodes — ***Kyra Yap***, *Jaime Aviles Acosta, Myles A. Steiner, Emily Warren, Adam Nielander, Thomas Jaramillo*

2:18 Paper 707g: Janus Heterostructured Bi-Cu_2s Nanocrystals for Efficient CO_2 Electroreduction to Formate — ***Xue Han***, *Tianyou Mou, Hongliang Xin, Huiyuan Zhu*

2:36 Paper 707h: Genetic Algorithm Organic Photoredox Catalyst Evolution for Efficient CO_2 Reduction and Degradation Resistance — ***Kareesa Kron***, *Andres Rodriguez-Katakura, Pranesh Regu, Maria Reed, Rachelle Elhessen, Shaama Mallikarjun Sharada*

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(708) Hydrocarbon Conversion II: Oxidative processes for hydrocarbon conversion

Friday, Nov 18, 12:30 PM
Phoenix Convention Center, N-127A

Yizhi Xiang, Chair
Konstantinos Alexopoulos, Co-Chair

Sponsored by: Catalysis

12:30 Paper 708a: Oxidative Coupling of Methane (OCM) over Strontium-Doped Neodymium Oxide: Parametric Evaluations and the Effect of Water Addition — ***Faisal Alahmadi***, *Anastasiya Bavykina, Daria Poloneeva, Adrian Ramirez, Robert Schucker, Jorge Gascon*

12:48 Paper 708b: Selective Epoxidation of Propylene on Promoted Ag/$CaCO_3$ catalysts — ***Joseph Esposito***, *Aditya Bhan*

1:06 Paper 708c: Density Functional Theory (DFT) Exploration of *Cs* & *Re* Promoter Effects on *Ag* Catalysts for Ethylene Oxidation — ***Adhika Setiawan***, *Tiancheng Pu, Israel Wachs, Srinivas Rangarajan*

1:24 Paper 708d: Partial Oxidation of Methane to Methanol over the Small-Pore Zeolite Cu-SSZ-39 — ***Jeewan Pokhrel***, *Daniel Shantz*

1:42 Paper 708h: First Principles Analysis of Oxidative Dehydrogenation of Ethane on Iron Sulfide Catalysts Using Sulfur As a Soft Oxidant — ***Anik Biswas***, *Yinan Xu, Allison Arinaga, Tobin J. Marks, Jeffrey Greeley*

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(709) New Developments in Computational Catalysis: Physics-Based Methods

Friday, Nov 18, 12:30 PM
Phoenix Convention Center, N-127B

Alexander Mironenko, Chair
Luke Roling, Co-Chair

Sponsored by: Catalysis

12:30 Paper 709f: Efficient Predictions of Methane Steam Reforming Pathway Energetics — ***Sarah Stratton***

12:50 Paper 709b: Towards Efficient Direct Dynamics Studies of Chemical Reactions: A Novel Matrix Completion Algorithm — *Stephen Jon Quiton, Jeongmin Chae, Selin Bac, Kareesa Kron, Urbashi Mitra,* ***Shaama Mallikarjun Sharada***

1:10 Paper 709c: A Combined Classical MD and DFT Approach for Modeling Ionic Adsorption on Metal Electrodes with Explicit Description of the Electrical Double Layer. — ***Bolton Tran***, *Andrew Wong, Scott T. Milner, Michael J. Janik*

1:30 Paper 709d: Microkinetic Modeling with Blowers-Masel Approximation to Scale Activation Energy Based on Enthalpy Change — ***Chao Xu***, *Richard H. West*

1:50 Paper 709g: Elucidating the Dependence of Nanoparticle Stability & Reactivity Metrics on the Choice of Exchange Correlation Functionals Using a Data Driven Approach — ***Asmee Prabhu***, *Jaideep Soodan, Verena Streibel, Joakim Halldin Stenlid, PhD, Frank Abild-Pedersen, Tej Choksi*

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(710) Nitrogen Chemistry: Nitrate and ammonia chemistry

Friday, Nov 18, 12:30 PM
Phoenix Convention Center, N-127C

Joseph Gauthier, Chair
Mutiu Amosa, Co-Chair
Aayush Singh, Co-Chair

Sponsored by: Catalysis

12:30: Break

12:48 Paper 710c: The Effect of N* Coverage on the Electrocatalytic Oxidation of Ammonia on Pt(111): Insights from Theory — ***Roberto Schimmenti***, *Saurabh Bhandari, Manos Mavrikakis*

1:06 Paper 710d: High-Performance Electrocatalytic Nitrate Reduction to Ammonia on Ordered Intermetallic Cupd Nanocubes: Breaking Adsorption-Energy Scaling Limitations — ***Qiang Gao***, *Hemanth Pillai, Hongliang Xin, Huiyuan Zhu*

1:24 Paper 710e: Electrochemical Synthesis of Urea By the Co-Reduction of Nitrates and CO2 on Co-Cu Bimetallic Gas Diffusion Electrodes (GDE) — ***Nishithan Balaji Chidambara Kani***, *Meenesh Singh*

1:42 Paper 710f: Molecular Electrocatalysis for Electrochemical Ammonia Recovery from Wastewater Nitrate — ***Matthew Liu***, *Dean Miller, William Tarpeh*

2:00 Paper 710g: Elucidating the Role of Oxygen and Hydrogen in the Early Elementary Steps of Nitrate Reduction — ***Michael T. Tang***, *Joakim Halldin Stenlid, PhD, Jinyu Guo, Elizabeth Corson, Matthew Liu, William Tarpeh, Frank Abild-Pedersen*

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(711) The Industrial Fluid Properties Simulation Challenge

Friday, Nov 18, 12:30 PM
Phoenix Convention Center, N-222B

Jonathan Moore, Chair
Daniel Siderius, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

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(712) Thermodynamics of Biomolecular Folding and Assembly

Friday, Nov 18, 12:30 PM
Phoenix Convention Center, N-222C

Gul H. Zerze, Chair
Diwakar Shukla, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

12:30 Paper 712a: Critical Evaluation of Implicit Solvent Hydration Free Energies from EEF1, Absinth, and GB/SA Versus Explicit Solvent Molecular-QCT Calculations — ***Rohan Adhikari Sridhar***, *Arjun Valiya Parambathu, Dilip Asthagiri, Walter Chapman*

12:45 Paper 712b: Physics-Based Modeling of Chromosomal Organization Impacted By Multiple Epigenetic Factors — ***Joseph Wakim***, *Sedona Murphy, Alistair Boettiger, Andrew Spakowitz*

1:00 Paper 712d: Protein-Polyelectrolyte Assembly: Influence on Structural Stability — *Kevin Moses,* ***Paul Van Tassel***

1:15 Paper 712e: Simulating Self-Assembly of Key Fragments on the α-Synuclein N-Terminal Using Discontinuous Molecular Dynamics Simulations — ***Van Nguyen***, *Carol Hall, Sheena E. Radford, David Brockwell, Sabine Ulamec*

1:30 Paper 712f: How Does Foldamer Side Chain Entropy Affect Folding Cooperativity? — ***Christopher Walker***, *Theodore Fobe, Sarah Mellett, Michael Shirts*

1:45 Paper 712g: The Transition State for the Growth of the Three-Fold Polymorph of Amyloid-β Fibrils Is Supported By Native Contacts — ***Sima Mafimoghaddam***, *Yuechuan Xu, Ted Kim, Peter Vekilov*

2:00 Paper 712h: Identifying Key Interactions in Amylin Self-Assembly Via Discontinuous Molecular Dynamics — ***Xin Dong***, *Carol Hall*

2:15 Paper 712i: String Method Based Free Energy Calculations Reveal the Role of Membrane Cholesterol in Bacterial Toxin Activity — ***Avijeet Kulshrestha***, *Sudeep Punnathanam, K. G. Ayappa*

2:30 Paper 712j: Graph Network Analysis of Protein-Osmolyte Preferential Interactions — ***M. Hamsa Priya***

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(713) Protein Assemblies and Aggregates

Friday, Nov 18, 12:30 PM
Phoenix Convention Center, N-125A

Benjamin S. Schuster, Chair
Yeongseon Jang, Co-Chair

Sponsored by: Bioengineering

12:30 Paper 713a: A High-Throughput Screen for Bacterial Microcompartment Closure — ***Carolyn E. Mills***, *Nolan W. Kennedy, Curt Waltmann, Monica Olvera De La Cruz, Danielle Tullman-Ercek*

12:48 Paper 713b: Surface Functionalization of Recombinant Barley Stripe Mosaic Virus-like Particles for Biomedical Applications & Nanomaterial Synthesis — ***Akash J. Vaidya***, *Julia Donlevie, Oluwatoni Akin-Adenekan, Kevin Solomon*

1:06 Paper 713c: Incorporation and Assembly of a Light-Emitting Enzymatic Reaction into Model Protein Condensates — ***Muyang Guan***, *Mikael V. Garabedian, Marcel Leutenegger, Benjamin S. Schuster, Matthew C. Good, Daniel A. Hammer*

1:24 Paper 713d: Structure Modeling and Design of Coiled-Coil Protein Origami — *Ratnakshi Mandal, Mostafa Bedewy,* ***Won Min Park***

1:42 Paper 713e: Assembly of a Modular and Tunable Worm-like Protein Nanostructure Using a Bottom-up Approach — ***Antonio Goncalves***, *Wilfred Chen, Millicent O. Sullivan*

2:00 Paper 713f: Microbially Synthesized Polymeric Amyloid Fiber Promotes β-Nanocrystal Formation and Displays Gigapascal Tensile Strength — ***Jingyao Li***, *Fuzhong Zhang*

2:18 Paper 713g: Design of Protein Nano-Architectures As Genetically Programmable, Functional Biomaterials — ***Claudia Schmidt-Dannert***

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(714) Advancing Chemical Engineering Education – Perspectives from the National Academies (Workshop)

Monday, Nov 14, 8:00 AM
Phoenix Convention Center, W-105C

Monica Lamm, Chair
Jodie Lutkenhaus, Co-Chair

Sponsored by: Education

8:00: Introductory Remarks

8:20: Discussion

9:20: Concluding Remarks

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(715) Combining Simulation and Machine Learning for the Optimization of Powder Handling Processes with Altair Solutions

Tuesday, Nov 15, 12:30 PM
Phoenix Convention Center, N-129AB

Erik Veikle, Chair

Sponsored by: Sponsored Technology Workshops

12:30 Paper 715a: Combining Simulation and Machine Learning for the Optimization of Powder Handling Processes with Altair Solutions — ***Erik Veikle***

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(716) Beyond the Optimizer: Gurobi's Hidden Gem Features and Applications in the Chemical Industry

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-124AB

Cara Touretzky, Chair

Sponsored by: Sponsored Technology Workshops

3:30 Paper 716a: Beyond the Optimizer: Gurobi's Hidden Gem Features and Applications in the Chemical Industry — ***Cara Touretzky***

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(717) Particle mechanics and solids handling in the process industries

Wednesday, Nov 16, 9:30 AM
Phoenix Convention Center, N-229AB

Ahmad Haidari, Chair

Sponsored by: Sponsored Technology Workshops

9:30 Paper 717a: Particle mechanics and solids handling in the process industries — ***Ahmad Haidari***

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(718) Combined In-Silico & Experimental Approach for Solid Form Crystallization Development

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, N-129AB

Yuriy Abramov, Chair
Shanming Kuang, Co-Chair

Sponsored by: Sponsored Technology Workshops

3:30 Paper 718a: Combined In-Silico & Experimental Approach for Solid Form Crystallization Development — ***Yuriy Abramov***, *Shanming Kuang*

(719) Chemical recycling, a big step toward a smaller footprint

Tuesday, Nov 15, 9:30 AM
Phoenix Convention Center, N-124AB

Jayme Leita, Chair

Sponsored by: Sponsored Technology Workshops

9:30 Paper 719a: Chemical recycling, a big step toward a smaller footprint — ***Jayme Leita***

(719) Wednesday LGBTQ+ & Allies Safe Zone Workshop

Wednesday, Nov 16, 10:30 AM
Phoenix Convention Center, N-226A

Anthony Butterfield, Chair

Sponsored by: LGBTQ+ and Allies Community

(720) RAPID Roadmapping: Critical Materials

Monday, Nov 14, 9:30 AM
Phoenix Convention Center, N-221B

Michelle Bryner, Chair
Sarah Ewing, Co-Chair

Sponsored by: RAPID

(721) RAPID Roadmapping: Hydrogen

Tuesday, Nov 15, 9:30 AM
Phoenix Convention Center, N-226A

Michelle Bryner, Chair
Sarah Ewing, Co-Chair

Sponsored by: RAPID

(722) RAPID Roadmapping: Food

Wednesday, Nov 16, 9:30 AM
Phoenix Convention Center, N-221C

Michelle Bryner, Chair
Sarah Ewing, Co-Chair

Sponsored by: RAPID

(723) RAPID Roundtable: Decarbonizing the Process Industries (I): Fuels and Chemicals

Sunday, Nov 13, 5:00 PM
Phoenix Convention Center, N-221C

Michelle Bryner, Chair
Sarah Ewing, Co-Chair

Sponsored by: RAPID

(724) RAPID Roundtable: Decarbonizing the Process Industries (II): Wastewater, Cement, Food & Beverage, and Pulp & Paper

Wednesday, Nov 16, 3:30 PM
Phoenix Convention Center, N-221B

Michelle Bryner, Chair
Sarah Ewing, Co-Chair

Sponsored by: RAPID

(726) How can advanced process technology support environmental justice?

Tuesday, Nov 15, 3:30 PM
Phoenix Convention Center, N-131A

Michelle Bryner, Chair
Sarah Ewing, Co-Chair

Sponsored by: RAPID

(727) Developing Industry Ready Skillsets for Engineers

Wednesday, Nov 16, 8:00 AM
Phoenix Convention Center, N-224AB

Walter Coto, Chair

Sponsored by: Sponsored Technology Workshops

8:00 Paper 727a: Developing Industry Ready Skillsets for Engineers — ***Walter Coto***

(728) Scale down first, before you scale up - a take on scale up of industrial microbial fermentation process

Monday, Nov 14, 5:00 PM
Phoenix Convention Center, N-124AB

Sangram Yadav, Chair

Sponsored by: Sponsored Technology Workshops

5:00 Paper 728a: Scale down first, before you scale up - a take on scale up of industrial microbial fermentation process — ***Sangram Yadav***

(729) Computational Chemistry Workloads via HPC Built for the Cloud

Tuesday, Nov 15, 8:00 AM
Phoenix Convention Center, N-124AB

Clinton Smith, Chair

Sponsored by: Sponsored Technology Workshops

8:00 Paper 729a: Computational Chemistry Workloads via HPC Built for the Cloud — ***Clinton Smith***

(732) RAPID Poster Session

Monday, Nov 14, 5:00 PM
Phoenix Convention Center, W-301 A

Julia Faeth, Co-Chair
Patricia Gillenwater, Co-Chair
Cody Hirashima, Co-Chair

Sponsored by: RAPID

Poster 732a: Spatial and Temporal Intensification of Poultry Processing Wastewater Treatment Units Using Stainless Steel Ultrafiltration Membrane — ***Saubana Dada***, *Mahmood Gheni Jebur, Ranil Wickramasinghe*

Poster 732b: Intensified CO2-to-Ethylene Process in Electrochemical Cells at Elevated Temperatures (350-500 °C) — ***Lucun Wang***, *Min Wang, Yingchao Yang, Dong Ding*

Poster 732c: Thermodynamic Modeling of Double Azeotrope - a Study of Methanol-Diethylamine Binary Mixture — ***Nooram Anjum***, *Shigeo Oba, Toshihiko Hiaki, Chau-Chyun Chen*

Poster 732d: Enhanced Liquid-Liquid Separation Using a 3D-Printed 2-Dimensional Device with Advanced Coatings — ***Lei Li***, *Aigerim Baimoldina, Fan Yang, Yihan Song, Cliff Kowall, Glenn Cormack*

Poster 732e: Efficient Chemicals Production Via Chemical Looping — ***Sunkyu Kim***, *Jian Pan, Arun Senthil Sundaramoorthy, Raul Lobo*

Poster 732f: Development and Demonstration of Novel Thermal Technologies for Enhanced Air - Side and Two - Phase Performance of Cpi - Relevant Heat Exchangers — ***Matthew Realff***, *Ari Glezer, Srinivas Garimella, Arne Pearlstein, Thomas Lestina*

Poster 732g: Microwave Catalysis for Process Intensified Modular Production of Value-Added Chemicals from Natural Gas — ***Brandon Robinson***, *Ashley Caiola, Yifan Deng, Sanjana Karpe, Dushyant Shekhawat, Joseph B. Powell*

Poster 732h: Integrating Reaction and Separation in a Thin Film Evaporator for Intensified Production of Dispersants — ***Riddhesh Patel***, *Nasser Al Azri, Hari Mantripragada, Nicolas Proust, Glenn Cormack, Robert M. Enick, Goetz Veser*

Poster 732i: Modelling for Optimal Operation of Modular Integrated Methane Dehydroaromatization Process — ***Arun Senthil Sundaramoorthy***, *Sunkyu Kim, Babatunde A. Ogunnaike, Raul Lobo*

Poster 732j: Process Modeling and Simulation of Electrochemical Processes Poster — ***Sadia Saberin***, *Chau-Chyun Chen*

Poster 732k: Argonne Capabilities in Chemical Process Intensification — ***Aaron Fluitt***, *Meltem Urgun-Demirtas*

Poster 732l: Separation of H2 Using Fluorinated Polymer Membranes RAPID Project 6.9 — ***Abby Harders***, *Micah Welsch, Rajkumar Kore, Brian Laird, Kyle Camarda, Alan Allgeier, Mark B. Shiflett*

Poster 732m: Optimizing Absorption to Improve Haber-Bosch Synthesis Poster — ***Alon McCormick***, *Cory Marquart, Chinomso Onuoha, Matthew Palys, Zac Pursell, Edward L Cussler, Prodromos Daoutidis, Paul Dauenhauer, Michael Reese, Sameer Parvathikar, Mahdi Malmali*

Poster 732n: Unlocking the Power of Sewage Sludge and Biosolids through the Integration of Supercritical Water Technologies to Produce Renewable Natural Gas — ***David Kenney***, *Geoffrey Tompsett, Michael R. Thorson, Jesse Bond, Michael T. Timko, Ignasi Palou-Rivera, Andrew R Teixeira*

Poster 732o: Deducing Subnanometer Heterogeneous Supported Catalyst Structure from Infrared Spectroscopy — ***Vinson Liao***, *Maximilian Cohen, Yifan Wang, Dionisios Vlachos*

Poster 732p: Facilitating Batch to Flow Process Conversion through Hands-on Training on Heat and Mass Transfer Characterization, Multiphasic Systems, and Microfluidic Equipment — ***Fatou Baka Diop***, *Ashli Silvera, Gabriela Chong, Andrew R Teixeira*

Poster 732q: Physical Property Data and Models in Support of Bioprocessing Separation Technologies for Organic Acids Separation — ***Meltem Urgun-Demirtas***, *Ignasi Palou-Rivera, Chau-Chyun Chen, Lauren Valentino, Simon Leyland, Jean Yves Delannoy*

Poster 732r: Modeling the Distribution of Supported Sub-Nanometer Cluster Catalysts Poster — ***Salman A. Khan***, *Stavros Caratzoulas, Dionisios Vlachos*

Poster 732s: Integrated Electrocoagulation/Ultrafiltration-Membrane Distillation-Crystallization for Treating Hydraulic Fracturing Produced Water — ***Ranil Wickramasinghe***, *Mahmood Gheni Jebur, Yelyzaveta Bachynska*

Poster 732t: Towards a Software Prototype for Synthesis of Operable Process Intensification Systems — ***Moustafa Ali***, *Navya Pabba, Shivam Vedant, Dustin Kenefake, Efstratios N. Pistikopoulos*

Poster 732u: Wirelessly Detect COVID Viruses, Bacteria, and Cells on Graphene Flakes-Improved Nano-Biosensor — ***Ryan Tian***, *Yang Tian, Ruqaiza Muhyudin, Priyangi Malaviarachchi, Roger Pechous, Xuming Zhang, John Hemmerling, Amy McCleney, Michael A. Miller, Linh Le, Steve Kaufman, Phil van Wormer, Brad Larschan, Erika Wojack, Patricia Gillenwater*

Poster 732v: Scale-up of Continuous Manufacturing and Productization of Graphene for Advanced Respirator and Biosensor Applications — ***John Hemmerling***, *Amy McCleney, Michael A. Miller, Phil van Wormer, Brad Larschan, Linh Le, Steve Kaufman, Ryan Tian, Patricia Gillenwater*

Poster 732w: Help to Transform the Process Industries: Join the RAPID Manufacturing Institute — ***Ashley Smith-Schoettker***

Poster 732x: Developing Future Leaders of the Process Industry: Nominate a RAPID Intern — ***Ashley Smith-Schoettker***

Poster 732y: Help Define Needs of the Current and Future Workforce: Virtual Technician and Operator Training Program — ***Ashley Smith-Schoettker***

Poster 732z: Accelerated Modular Process Development for Domestic Manufacturing of Critical Pharmaceutical Precursors — ***Nima Yazdanpanah***, *Cheryl Teich, John Dever, Mike Burgess, Robert Nunley, Ignasi Palou-Rivera, Patricia Gillenwater*

Poster 732aa: Process Intensification of Drying of Paper and Biomaterials: Experimental Analysis of Convective Drying — ***Sridharan Ramaswamy***, *Koushik Sampath, Leonard Reynolds, Michael Ringold, Xinyi Li, Huajiang Huang*

Poster 732ab: Design and Development for Functionality, Manufacture and Market of Modular Multi-Phase Extraction and Separation — ***Francis Chukwunta***, *Jad Touma, Lucas Freiberg, Matthew Coblyn, Goran Jovanovic, Cliff Kowall, Lei Li*

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(733) How to Maintain Productivity in a Crisis

Monday, Nov 14, 3:30 PM
Phoenix Convention Center, N-122B

Alaina Levine, Chair

Sponsored by: Miscellaneous

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(734) Networking for Nerds: Find and Forge Relationships that Deliver ROI for All

Monday, Nov 14, 4:45 PM
Phoenix Convention Center, N-122B

Alaina Levine, Chair

Sponsored by: Miscellaneous

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(735) Café with LatinXinChE

Wednesday, Nov 16, 11:00 AM
Phoenix Convention Center, W-102C

Gabriel Rodriguez, Chair
Sindia M. Rivera-Jimenez, Co-Chair

Sponsored by: Minority Affairs Committee (MAC)

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(736) Unconscious Bias II

Monday, Nov 14, 9:30 AM
Phoenix Convention Center, N-226B

Eric Bell, Chair
Bryan Deschamps, Co-Chair

Sponsored by: Engineering for Inclusion

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(737) Siemens Sponsored Technology Workshop

Wednesday, Nov 16, 5:00 PM
Phoenix Convention Center, N-124AB

Sponsored by: Sponsored Technology Workshops

Accurate as of Monday, November 7, 2022