2021 AIChE ANNUAL MEETING

NOVEMBER 7-11 • BOSTON, MA

NOVEMBER 15-19 • VIRTUAL

Building the Bridge in 21st Century Education:
Chemical Engineering Industry + Academia

2021 AIChE ANNUAL MEETING TECHNICAL SESSIONS

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

Sunday, Nov 7, 1:00 PM
John B. Hynes Veterans Memorial Convention Center, Exhibit Hall C/D

Sundararajan Madihally, Chair
Roman Voronov, Co-Chair

Sponsored by: Meet the Candidates Poster Sessions

Poster 4a: Process Intensification of Combined Carbon Capture and Utilization Using Multi-Functional Materials and Catalysts — ***Chae Jeong-Potter***
Poster 4c: Encapsulation and Stabilization of Biomolecules and Modeling Polymer Depolymerization — ***Whitney Blocher McTigue***
Poster 4d: Modeling of Soft Materials: *Model-Driven Versus Data-Driven*— ***Shiyan Wang***
Poster 4e: Characterizing the Mechanical and Transport Properties of Crosslinked Poly(vinyl alcohol)–Lignin Soft Composites for Membrane-Based Separations — ***Nicholas Gregorich****, Graham Tindall, Sagar Kanhere, Jaden Stutts, Junhuan Ding, Tyler Martin, Amod Ogale, Mark Thies, Eric M. Davis*
Poster 4f: Platform Technologies for Biomarker Signature Discovery and Personalized Diagnostics — ***Connie Wu***
Poster 4g: Templated Crystallization: An Emerging Nanofabrication Strategy for Naturally Derived Biopolymers — ***Hui Sun****, Benedetto Marelli*
Poster 4h: Machine-Aided Design and Manufacturing of Polymeric Materials— ***Weizhong Zou***
Poster 4i: Genome Engineering and Systems Biology Tools for Probing Endo-Lysosomal Pathophysiology to Develop Novel Therapeutics — ***Vivek Bajpai, MD, PhD***
Poster 4k: Active Learning for Surrogate Model Design in Superstructure Optimization — ***Julia Granacher****, Ivan D. Kantor, François Maréchal*
Poster 4l: Symmetry Breaking in Optical Nanomaterials. — ***Ji-Young Kim***
Poster 4n: Self-Assembly of Evolvable and Functional Colloidal Polymeric Materials — ***Angus McMullen***
Poster 4o: Electrokinetic Transport of Nanoparticles through Micro and Nanochannels — ***Siamak Mirfendereski****, Justin Brooks, Ruiguo Yang, Jae Sung Park*
Poster 4p: Designing Nanoscale Hybrid Materials for Reactive Separation of CO_2 and Critical Elements to Build a Sustainable Future — ***Guanhe Rim***
Poster 4s: Uncovering and Enhancing Intrinsic Characteristics of Proteins for Novel Applications — ***Leah Spangler***
Poster 4t: Designing Protein-Based Biomaterials for Biomedical Applications— ***Jessica Torres***
Poster 4u: Reducing Carbon Footprint *Via* Electrochemistry and Materials Design — ***Fang Liu***
Poster 4v: Advancing Organic Macromolecular Chemistry through the Development of Functional, Sustainable and Responsive Materials — ***Wontae Joo***
Poster 4w: Device and Materials Physics of Emerging Semiconductors for Renewable Energy and Low-Cost Optoelectronics — ***Nolan M. Concannon****, Russell J. Holmes*
Poster 4x: Clonally Expanded, GPR15-Expressing Effector Th2 Cells Are Associated with Eosinophilic Esophagitis — ***Duncan Morgan***
Poster 4y: *Freedom*: First-Principles Aided Reverse Engineered Design of Materials — ***Abhinav Sankara Raman***
Poster 4z: Rare Earths and Computational Techniques — ***Richard Shiery***
Poster 4aa: Modeling the Human Blood-Brain Barrier: Leveraging *in Vitro*Models for the Identification of Novel Brain Targeting Antibodies — ***Moriah Katt***
Poster 4ab: Mathematical Modeling in Water Network Resilience and Pharmaceutical Process Optimization — ***Daniel Laky***
Poster 4ac: Leveraging Soft Matter Transport and Biomolecular Interactions to Transform Human Health — ***Aditya Raghunandan***
Poster 4af: A Sustainable Future for Manufacturing: Enabling Scalable Manufacturing of Polymeric Materials in Synergy with Educational Initiatives— ***Cecile Chazot****, A John Hart*
Poster 4ag: Leveraging Chemical, Physical, and Engineering Approaches for Functional Polymers — ***Alexa Kuenstler***
Poster 4ai: Engineering Models in Gut-Organ Axes: Immunity, Infection and Nanomaterial Therapeutics for Improved Healthcare — ***Mohammad Aminul Islam***
Poster 4aj: A Systems-Level Approach to the Design of Sustainable Processes— ***Juan Manuel Restrepo-Florez***
Poster 4ak: Adaptable Polymer Networks with Enabling Properties — ***Matthew McBride***
Poster 4al: Model-Based Design of Pharmaceutical Crystallization Processes— ***Ayse Eren***
Poster 4am: Extending a Microfluidic Platform to Elucidate Bacterial Communication in Humans Its Impact on Disease — ***Corine Jackman***
Poster 4an: Multiscale Modeling for Hierarchical Materials Design — ***Xin Qi***
Poster 4ao: Mechanics of Bio-Inspired Soft Responsive Coatings — ***Bavand Keshavarz***
Poster 4aq: Simulations of Chemical Signaling and Homeostasis in Neurological Systems — ***Mackenzie Clay***
Poster 4ar: Microstructure and Rheology of Rod-like Viruses at High Shear Rates Via Capillary Rheo-SANS — ***Steve Kuei****, Paul F. Salipante, Ryan P. Murphy, Katie Weigandt, Steven D. Hudson*
Poster 4as: Development of Nanozyme-Linked Immunosorbent Assays— ***Eunice Kwon***
Poster 4au: Developing Intelligent High Surface Area Catalysts with Atomic Layer Deposition — ***Tzia Ming Onn****, Raymond J. Gorte, Paul Dauenhauer*
Poster 4av: Computational Design of Bimolecular Self-Assembly and Adsorption Behaviors through Thermodynamically Consistent Multiscale Modeling — ***Jacob I. Monroe***
Poster 4aw: Novel Thin Film Deposition Techniques to Accelerate Data-Driven Discovery and Optimization of Optoelectronic Hybrid Organic-Inorganic Materials — ***Wiley Dunlap-Shohl***
Poster 4ax: Deterministic Optimization of Hybrid Models for Advanced Manufacturing Systems — ***Matthew Wilhelm***
Poster 4ay: Accurate and Efficient Thermodynamic Approach to Evaluate Molecular Adsorption and Diffusion in Nanoporous Materials — ***Musen Zhou***
Poster 4bb: Engineering Active Materials — ***John Berezney***
Poster 4bc: Scalable Nanomanufacturing of Multifunctional Materials for Sustainable Environment — ***Sooyoun Yu***
Poster 4bd: Dynamic Catalysis over Mixed Metal Oxides for Clean Energy and Sustainability — ***Debtanu Maiti***
Poster 4bg: Ionic Dissociation and Ionic Conductivity in Model Thin Film Polymer Electrolytes — ***Mario Ramos-Garces***
Poster 4bh: Integrating Circular Hydrogen and Carbon Economies Via Molecular Design of Hybrid Functional Materials Utilizing Innovative Energy Carriers — ***Hunter Vibbert***
Poster 4bi: Bridging the Protein-Polymer Divide: Designer Protein Materials with Programmed Dispersity — ***Melody Morris***
Poster 4bj: Postdoc Candidate: Mammalian Genome Engineering for Discovery of Novel DNA Regulatory Elements — ***Meng Zhang***
Poster 4bk: Engineering Microbiomes and Diet to Promote Health — ***Matthew Ostrowski***
Poster 4bl: Data-Driven Optimization Methods for the Design and Operation of Low-Carbon Energy and Chemical Production Systems — ***Ishan Bajaj***
Poster 4bm: Designing Structures and Functions of Soft Materials By Tuning Interactions — ***Chrisy Xiyu Du***
Poster 4bo: Interfacial Engineering of Next Generation Colloidal Nanomaterials for Energy, Sustainability, and Health Applications — ***Dorsa Parviz***
Poster 4bp: Big Data + Machine Learning + Mechanistic Models = Mechanistic Precision Medicine — ***Cemal Erdem***
Poster 4bq: Investigating the Tumor Microenvironment through State-of-the-Art DNA-Based Technology — ***Molly Kozminsky****, Lydia L. Sohn*
Poster 4br: Biohybrid Responsive Materials for Cell-like Behavior — ***Alexander Marras***
Poster 4bs: Understanding Complexity in Membrane Systems for Efficient Separations and Advanced Energy Technologies — ***Daniel Miller***
Poster 4bt: Leveraging Multiscale Modeling to Address Future Fuel and Chemical Needs — ***Pavlo Kostetskyy***
Poster 4bu: Electrochemically Active ZnO Formed in Rechargeable Zinc Alkaline Batteries: Mechanistic Insights for Improved Zinc Battery Performance— ***Brendan Hawkins****, Damon E. Turney, Robert Messinger, Gautam Yadav, Sanjoy Banerjee, Andrew M. Kiss, Timothy N. Lambert*
Poster 4bv: Integrating Environmental Economics into Supply Chains with Systems Engineering Approaches — ***Philip Tominac***
Poster 4bw: Thermo-Mechanics for Energy and Environmental Applications— ***Michela Geri***
Poster 4bx: Novel Titania Based Composites for Solar Disinfection — *Ashleigh Fletcher,* ***Anam Safri***
Poster 4by: Expanding Symbiotic Nitrogen Fixation — ***Cheryl Immethun***
Poster 4bz: Renewable Polymers and the Design of Sustainable Plastics— ***Wui Yarn Daphne Chan***
Poster 4cb: Interfaces in Thermal-Catalysis and Electro-Catalysis: Methodological and Conceptual Challenges in Connecting Two Worlds— ***Arthur Shih***
Poster 4cc: Computation and Theory of Materials with New Quantum Properties— ***Elizabeth M.Y. Lee***
Poster 4cd: Leveraging Electrostatic Interactions to Enhance Drug Delivery through Tumor Extracellular Matrix — ***Rashmi Mohanty***
Poster 4ce: Electromagnetic Fields to Drive Assembly and Transport in Colloidal Soft Materials — ***Zachary Sherman***
Poster 4cf: Advancing Future Manufacturing By Integrating Experimental and Computational Data with Machine-Learning (ML)-Based Frameworks — ***Hud Wahab***
Poster 4cg: A Dynamical Systems Approach to Active Matter Design and Control — ***Michael Norton***
Poster 4ci: Development of Catalysts for Environmental Remediation and Clean Energy Applications — ***Musa Najimu***
Poster 4cj: Dissecting and Designing (electro)Catalytic Interfaces with Atomically Precise Motifs — ***Joy Zeng***
Poster 4ck: Design of Advance Materials By Using *Ab Initio*structural Search— ***Irais Valencia Jaime***
Poster 4cl: First-Principles Design of Materials for Catalysis and Separations— ***Daniel Schwalbe-Koda***
Poster 4cn: Towards Practical Quantum Applications Via Defect Engineering in Two-Dimensional Materials — ***Sylvia Xin Li***
Poster 4co: Could We 3D Print a Light Bulb at Home? 2D Nanomaterials Used for 3D Printing, Biosensing, and Control Release of Intercalates — ***Deisy Cristina Carvalho Fernandes***
Poster 4cq: Capture and Conversion of CO_2 – Towards CO_2 Recycling— ***Juliana Carneiro***
Poster 4cr: Interfacial and Rheological Properties of Ocular Epithelia — ***Chunzi Liu****, Gerald Fuller*
Poster 4cs: Development of Microbial Hosts for Low-Cost Manufacturing of Vaccines and Therapeutic Proteins — ***Neil Dalvie***

Poster 4ct: Converting Waste to Value Added Products: Thiol-Functionalized Hyper-Cross-Linked Milk Protein Polymers for Mercury Removal — ***Maryam Davaritouchaee****, Ahmadreza Khosropour, Alireza Abbaspourrad*

Poster 4cu: Engineering Functional Biomaterials and Smart Delivery Systems for Gene Therapy — ***Jayoung Kim***

Poster 4cv: Directing Amyloid-β Structural Polymorphism: The Relationship between Fibril Structure and Phenotype — ***Henry Pan****, Michael Lucas, Eric Verbeke, Gina Partipilo, Benjamin K. Keitz, David W. Taylor, Lauren Webb*

Poster 4cw: Non-Linear Electrokinetics and Interfacial Microfluidics: Manipulating Molecules and Organisms on-Demand for Biomedical Science— ***Gongchen Sun***

Poster 4cy: Addressing Challenges of Chemical Engineering Education in a Virtual Learning Environment — ***Zachary Stillman****, Catherine Fromen*

Poster 4da: Multiscale Systems Engineering Frameworks for the Development of Sustainable Technologies — ***Elvis Eugene***

Poster 4db: Structure-Property Relationships in Edible and Nonedible Polymers— ***Karthika Suresh***

Poster 4dd: Energy-Efficient Functionalized Filters with Easily Accessible Materials for Nanoparticle Removal from Water — ***Laxmicharan Samineni***

Poster 4de: Computational Engineering Towards Sustainable High-Pressure Processing and Intelligent Characterization of Porous Materials — ***Kaihang Shi***

Poster 4dg: Bridging Atomistic and Experimental Scales in Electrochemistry for Energy Storage and Catalysis — ***Karun Kumar Rao***

Poster 4dh: Computational Biology in Research and Classrooms: From Modeling CAR T-Cells in Solid Tumors to Developing Educational Tools for Inclusive, Active Learning Environments — ***Alexis Prybutok***

Poster 4dk: Leveraging Statistical Inference and Physical Modeling to Augment Electrochemical Analysis of Charge Storage Materials — ***Alexis Fenton Jr.***

Poster 4di: Engineered Immune Cells with Nanoparticles for Advanced Combinatorial Cancer Theranostics and Post-Treatment Assessment— ***Jinhwan Kim***

Poster 4dl: Understanding and Controlling Multi-Scale Complex Fluid Flows— ***Charles Young***

Poster 4dp: Nanoparticle Tracking to Probe Transport in Porous Media— ***Haichao Wu***

Poster 4dq: Modulating Platelet-Cell and Platelet-Particle Dynamics in Blood Flow — ***Alison Banka***

Poster 4ds: Advanced Manufacturing of Functional Soft Matter for Environmental Sustainability and Energy-Efficiency — ***Sangchul Roh***

Poster 4dt: Combining Multiscale Modelling and Machine Learning to Design New Polymers and Biomolecules — ***Yaxin An***

Poster 4du: Computational Materials Chemistry for Energy Conversion and Storage Applications — ***Robert Warburton***

Poster 4dv: Surfactant Uses in Pulmonary Disease Treatment and Drug Delivery: Marangoni Transport, Dilatational Rheology, and Surfactant Adsorption— ***Steven Iasella***

Poster 4dw: Conversion of Renewable Waste to Value-Added Products By Microorganisms — ***Maryam Davaritouchaee***

Poster 4dx: Designing the Active Centers and Solvating Environments of Heterogeneous Catalysts for Energy, Organic Synthesis, and the Environment— ***Jason S. Bates***

Poster 4dz: Machine Learning for Systematic Material Design and Process Development in Vapor and Liquid-Based Crystallization — ***Hossein Salami***

Poster 4ea: Field Wide Optimisation Towards Improved Field Recovery— ***Shakeel Ramjanee***

Poster 4ec: Graphical Model Framework for Automated Annotation of Cell Identities in Dense Cellular Images — ***Shivesh Chaudhary****, Sol Ah Lee, Yueyi Li, Hang Lu*

Poster 4eb: Fluids-Based *in Vitro* Models for Development and Disease— ***Kiara Cui****, Leeya Engel, Vincent Xia, Kevin Liu, Daniel Cirera Salinas, David Myung, Kyle Loh, Lay Teng Ang, Alexander R. Dunn, Gerald Fuller*

Poster 4ed: Using Structure-Function Relationships to Engineer Therapeutics By Design — ***Michelle Teplensky***

Poster 4ee: High-Value Fuels and Chemicals from Renewable Feedstocks: A Catalytic Process Design Approach. — ***Gabriel Viana Sueth Seufitelli***

Poster 4ef: Integrate Machine Learning in Automated Quantum Chemistry Calculation Workflows: Towards Faster and More Accurate Chemical Discovery— ***Chenru Duan****, Heather Kulik*

Poster 4eg: Statistical Physics of Ionic Polymer Systems for Rational Materials Design — ***Artem Rumyantsev***

Poster 4eh: Materials for Separations: Development of Synthesis Methods for Novel Composite Materials and Their Performance Tuning By Vapor-Phase Processes — ***Dennis Lee***

Poster 4ei: Local Structure and Global Behavior in Self-Assembling, Amorphous, and Neurobiological Systems — ***Erin Teich***

Poster 4ej: Macromolecule-Mediated Ion Transport for Advanced Materials— ***Thomas Schroeder***

Poster 4ek: Materials for Energy, Mass and Information Transport — ***Xingfei Wei***

Poster 4el: Materials Processing and Structure Formation in Compositionally Inhomogeneous and Reactive Complex Fluids — ***Joseph Peterson***

Poster 4em: Molecular Simulations, Neural Networks, and Active Learning for Molecular Design — ***Camille Bilodeau***

Poster 4en: Novel Facilitated Transport Membrane and Process for Post-Combustion Carbon Capture — ***Yang Han****, W.S. Winston Ho*

Poster 4eo: Peptide-Functionalized Materials for Bioprocessing, Molecular Identification, and Drug Delivery — ***Nicholas Vecchiarello***

Poster 4ep: Process Intensification and Optimization of Energy Systems Towards a Sustainable Future — ***Zewei Chen***

Poster 4eq: Programming Structural Transition in Dynamic Systems — ***Yimin Luo***

Poster 4er: Rapid Self-Assembly: Biomimetic Membranes from Membrane Protein-Block Copolymer Nanosheets — ***Yu-Ming Tu***

Poster 4es: Rational Design of Biointegrated Materials and Devices Towards Precise and Closed-Loop Bioelectronic Medicine — ***Yuanwen Jiang***

Poster 4et: Rational Design of Catalysts to Upgrade Plastic Waste and Sustainable Feedstocks — ***Julie Rorrer***

Poster 4eu: Molecular Structures of Solid-Confined Ionic Liquids and Their Applications As Media Lubricants in Hard Disk Drives — ***Bingchen Wang***

Poster 4ew: Solving the Next Generation of Transport Challenges in Electrochemically Mediated Processes — ***Kyle Diederichsen***

Poster 4ex: Study of Impact of Flexibility on Molecular Diffusion in MOFs— ***Yuhan Yang****, David Sholl*

Poster 4ey: Synthesizing and Optimizing Manganese Dioxide Nanorods and Its Behavior Toward Oxygenreduction Reaction — ***Abid Ullah****, Basharat Hussain, Sayed Sajid Hussain*

Poster 4ez: Using Atomistic Simulations and Machine Learning Technology to Discover New Porous Materials for Sustainable Energy Applications — ***Xiaoyu Wang***

Poster 4fa: *A Repackaged CRISPR/Cas9 Platform Recasts Non-Homologous End Joining As a Beneficial Instrument in Nonconventional Yeast Engineering*— ***Deon Ploessl****, Zengyi Shao*

Poster 4fb: Data Driven Discovery of Novel Functional Materials and Process Understanding — ***Aparajita Dasgupta***

Poster 4fc: Microwave-Assisted Heterogeneous Catalysis for Natural Gas Utilization — ***Xinwei Bai***

Poster 4fd: Tissue Interfacing Robotic Therapeutics — ***Alex Abramson***

Poster 4fe: RECAPS in the Chemical Engineering Classroom — ***Rebecca Harmon***

Poster 4ff: Engineering Chemical Tools for Autoimmune Modulation and Investigation — ***Peter Deak***

Poster 4fg: Decipher the Complexity of Natural Microbial Communities— ***Fangchao Song***

Poster 4fh: Silver Quantum Clusters Conjugated Polysaccharide Gum: A One-Pot Approach — ***Neelima Tripathi****, Sri Sivakumar*

Poster 4fi: Engineering Biopolymer Crystallinity in Microneedles for Improved Food Monitoring System — ***Doyoon Kim****, Benedetto Marelli*

Poster 4fj: Designing Advanced Biomaterials By Leveraging Advances in Macromolecular Engineering — ***Yongsheng Gao***

Poster 4fk: Understanding Electrochemical Systems across Length and Time Scales — ***Kara Fong***

Poster 4fl: Optimal Design and Control of Advanced Biomanufacturing Systems— ***Moo Sun Hong***

Poster 4fn: Confinement Effects in Self Assembly of Functional Block Copolymers — ***Jonathan Coote****, Joshua Sangoro, Gila E. Stein*

Poster 4fo: Electrochemical Techniques in Separation Processes — ***Ali Estejab***

Poster 4fq: Engineered Microenvironments to Assess the Potential of Idiosyncratic Toxic Events — ***Sophia Orbach***

Poster 4fs: In-Situ Spectroscopic Investigations to Understand the Behavior of Heterogeneous Catalysts — ***Sean Najmi***

Poster 4ft: Multi-Scale & Multi-Physics Computation Driven Process Intensification — ***Abhinav Malhotra***

Poster 4fv: Applications of Nonequilibrium Thermodynamics & Simulation— ***Alex Albaugh***

Poster 4fw: Osmotic-Capillary Principles for Microfluidic Pumping and Fluid Management for Sweat Lactate Sensing Devices — ***Tamoghna Saha***

Poster 4fx: Materials Design for Energy and Environmental Applications— ***Yuyin Xi***

Poster 4fy: Biodegradable Nanofiber Bone-Tissue Scaffold As Remotely-Controlled and Self-Powered Electrical Stimulator — *Thanh Nguyen,* ***Ritopa Das***

Poster 4fz: Complex Interfaces As the Future of Understanding Soft and Biological Matter — ***Joseph Barakat***

Poster 4ga: Engineering Biomaterials for Therapeutic Approaches — ***Gabriel Rodriguez-Rivera***

Poster 4gb: Synthetic Biology Mediated Applications of Electrochemical Biosensor and the Formation of Artificial Organelle in Living System — ***Yifan Dai***

Poster 4gc: Macrophage Engineering: From Enhancing Phagocytosis By Disrupting "Self" Signals to Cellular Immunotherapies and Tissue Patterning— ***Lawrence J. Dooling***

Poster 4gd: Molecular Engineering of Advanced Polymeric Materials for Energy and Sustainability — ***Anthony Engler***

Poster 4ge: Active Matter Coupled to Crystalline Defects Via Strain Field Optimization — ***Bryan VanSaders****, Sharon C. Glotzer*

Poster 4gf: Computational Biomolecular Discovery and Development — ***Matteo Aldeghi***

Poster 4gg: Electrochromic Voltage Imaging at Neural and Cardiac Interfaces: From Fundamentals to Applications — ***Yuecheng Zhou***

Poster 4gi: Fundamental Aspects of Surface Science and (Electro)Catalysis - Bridging the Atomic and Macro Scales — ***Joakim Halldin Stenlid, PhD***

Poster 4gj: Deciphering Immune Cell Signaling Pathways and Transcriptome Responses to Colorectal Cancer-Derived Extracellular Vesicles — ***Joshua Hinckley****, J. Christopher Love*

Poster 4gk: Aptamer Based Pesticide Detection: Tri-Element Analysis— ***Shalini Shikha****, Sudip Pattanayek*

Poster 4gl: Post-Doc Candidate: Leveraging Biomaterials for the Advancement of Women's Reproductive Health Research — ***Beverly Miller***

Poster 4gn: Process Systems Engineering for Sustainable Chemicals — ***Ana Somoza Tornos***

Poster 4go: Single-Sequence Protein Structure Prediction and Applications in Protein Design and Novel Biomaterials — ***Ratul Chowdhury***

Poster 4gp: Fast Prototyping, Additive Manufacturing, and Rheology: Designing Better Systems and Tooling — ***Crystal Owens***
Poster 4gt: Rationally Designed and Nanoengineered Functional Materials to Address Future Needs — ***Imann Mosleh, PhD***
Poster 4gu: Computational Explorations of Self-Assembly and Collective Dynamics in Living and Non-Living Systems — ***Kimberly Bowal***
Poster 4gv: Biomaterial-Driven Immune Modulation for Cancer and Autoimmune Diseases — ***Apoorv Shanker***
Poster 4gw: Employing Shape As a Handle for Materials Design — ***Thi Vo***
Poster 4gx: Dynamic Separation of Petrochemicals through Crystalline Sponges — ***Gonzalo Campillo-Alvarado***
Poster 4gz: Soft Materials for Membrane Separations for Water, Energy, and the Environment — ***Joshua Moon***
Poster 4ha: Theory-Guided Transformations of Inorganic Materials for Sustainable Energy Conversion and Storage — ***Christopher J. Bartel***
Poster 4hb: Data Driven Development of Approximate Inertial Forms and Closures for Coarse-Scale Modeling of Multiphase Flows — ***Cristina Martin Linares***
Poster 4hc: Engineering Nanostructured Soft Materials for Electrochemical Processes and Water Treatments — ***Zhongyang Wang***
Poster 4hf: Machine Learning and Computational Tools for Molecular Properties and Reaction Systems — ***Charles J. McGill***
Poster 4hg: Towards a New World of Plastic Processing & Recycling Via Advanced Reactor Technologies — ***Ali Zolghadr***
Poster 4hi: Material extrusion based additive manufacturing of semicrystalline polymers for multifunctional applications — ***Arit Das***, *Michael Bortner*
Poster 4hj: Development and Implementation of Enhanced Sampling Approaches:Applications to Ion-pairing in Battery Electrolytes and Nucleation ofNano-porous Materials — ***Ajay Muralidharan***, *J.R. Schmidt, Arun Yethiraj*
Poster 4hk: Scalable Nanomaterials: From Polymer Nanocomposites to Protein Therapeutics — ***Neha Manohar***
Poster 4hl: Synthesis-Structure Relationships in Plasma Modified Catalysts and Catalyst Synthesis — ***David Barlaz***
Poster 4hm: Microfluidic functional assays for assessing the roles of extracellular vesicles in microvascular ischemia-reperfusion and thromboinflammation — ***Ran An***, *Umut Gurkan*
Poster 4hn: Pushing the Frontier of Ionic Polymer Self Assembly and Processing — ***Angelika Neitzel***, *Yan Fang, Carlos Medina Jimenez, Boyuan Yu, Artem Rumyantsev, Guilhem De Hoe, Juan J. DePablo, Matthew V. Tirrell*
Poster 4ho: Automating Systems Engineering of *Smart and Eco-friendly*Synthetic Microbes — ***Chelsea Hu***
Poster 4hp: Modeling, Simulation and Optimization of Direct and Indirect Mineralization Strategies for CO_2 Capture — ***Rafael Castro-Amoedo***, *Mouhannad A. Daher, François Maréchal*
Poster 4hq: Development of chiral nanomaterials for translational medicine— ***Anastasiia Visheratina***
Poster 4hr: Bridging Decision-Making at the Microscopic and Macroscopic Levels using Heterogenous Modeling and Optimization — ***Calvin Tsay***
Poster 4hs: Soft Material Engineering for the Environment, Health, and Sustainability — ***Navid Bizmark***
Poster 4ht: Catalyst Synthesis and Fundamental Investigation of Electrochemical Reactions — ***Bjorn Hasa***
Poster 4hu: Molecular-based modeling of polymer dynamics for material design and processing — ***Marat Andreev***
Poster 4hv: Integrated Computational Approach for Accelerated Materials Discovery and Advancement — ***Pranab Sarker***
Poster 4hw: The Search for Novel Mesoscale Materials: Leveraging Physics-Inspired Machine Learning Representations for Multiscale Simulation — ***Rose Cersonsky***
Poster 4hx: Polymeric materials for biomedical applications — ***Wei Zhang***
Poster 4hy: Harness the structural complexity and synthetic accessibility of disordered energy materials using data driven approach — ***Bin Ouyang***

(5) Public Affairs and AIChE: A PAIC Town Hall

Sunday, Nov 7, 3:00 PM
John B. Hynes Veterans Memorial Convention Center, 303

Gayle Gibson, Chair
Martin A Abraham, Co-Chair

Sponsored by: Public Affairs and Information Committee (PAIC)

(6) 3D Printing Fundamentals and Applications

Sunday, Nov 7, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 202

Nese Orbey, Chair
William Phillip, Co-Chair

Sponsored by: 3D Printing

3:30: Introductory Remarks
3:55 Paper 6b: Influence of Interfaces in Electrical Properties of 3D Printed Structures — ***Fraser Daniel***, *Andy Gleadall,* ***Adarsh Radadia***
4:20 Paper 6c: Modeling Heat Transfer in Material Extrusion Additive Manufacturing: Balancing Model Resolution with Computational Demands— ***Michael Bortner***, *James T. Owens, Arit Das*
4:45 Paper 6d: Assessing the Fidelity of Additively Manufactured Objects— ***Hajar Taheri Afarani***, *Edward Garboczi, Newell H. Moser, Ebrahim Nasr-Esfahani, Joseph J. Biernacki*
5:10 Paper 6e: Design and Processing of Open Lattice Structures for Tunable Fluid Phenomena — ***Ian Woodward***, *Lucas Attia, Premal Patel, Catherine Fromen*
5:35 Paper 6f: Methods to Evaluate Residual Stress in FDM Printed Parts— ***Daniyal Shoukat***, *Connor Forte, Macrae Montgomery, Haley Hilborn, Jerry Qi, Nese Orbey*

(7) Advances in Biosensors, Protein Production, and Protein Engineering

Sunday, Nov 7, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 111

Shelby Mills, Co-Chair
Kevin Metcalf, Co-Chair

Sponsored by: Bioengineering

3:30 Paper 7a: Portable and Label-Free Quantitative Loop-Mediated Isothermal Amplification (qLAMP) for Reliable COVID-19 Diagnostics in 3 Minutes: An Arduino-Based System Assisted By a pH Microelectrode — ***Mario Moisés Álvarez***, *Grissel Trujillo de Santiago, Sergio Bravo-González, Everardo Gonzalez Gonzalez*
3:48 Paper 7b: Integration of Living Analytics into Biomanufacturing Processes— *Ignacio Moya Ramirez, Pavlos Kotidis, Masue Marbiah, Juhyun Kim, Cleo Kontoravdi,* ***Karen Polizzi***
4:06 Paper 7c: Genome-Wide Knockout Screens Reveal New Engineering Targets That Enhance Protein Secretion in a Non-Model Yeast — ***Neil Dalvie***, *Timothy Lorgeree, J. Christopher Love*
4:24 Paper 7d: Engineering Incorporation of Non-Standard Amino Acids in a Gram-Positive Bacterium — ***Aditya Kunjapur***
4:42 Paper 7e: Directed Evolution of Metalloproteinase Inhibitors Targeting ADAM-17 — *Mari Toumaian, Imam Sanousi, Catherine Dyer, Amelia Bryan,* ***Maryam Raeeszadeh Sarmazdeh***
5:00 Paper 7f: Auto-ASR: A Web Server Providing Automated High-Throughput Ancestral Sequence Reconstruction for Combinatorial Protein Library Design— ***James VanAntwerp***, *Patrick Finneran, Daniel Woldring*
5:18 Paper 7g: Transcriptional Programming - Engineering Decision Making in Biology — ***Corey Wilson***

(8) Applications of Data Science in Catalysis and Reaction Engineering I

Sunday, Nov 7, 3:30 PM
Marriott Copley Place, Salon H/I

Zachary Ulissi, Chair
Bryan Goldsmith, Co-Chair
Thomas Senftle, Co-Chair

Sponsored by: Applications of Data Science to Molecules and Materials

3:30 Paper 8a: Understanding Barrierless Adsorption in Electro-Catalytic Systems Using Accelerated Transition Path Sampling — ***Mayank Agrawal***, *Adam P. Willard, Andrew A. Peterson*
3:48 Paper 8b: Methods and Applications of *Ex-Machina* Molecular Dynamics to Catalytic Processes — ***Boris Kozinsky***
4:06 Paper 8c: Statistical Models for Predicting Oil Composition from Hydrothermal Liquefaction of Biomass — ***Seshasayee Mahadevan Subramanya***, *Nicholas Rios, Abbey J. Kollar, Rachel Stofanak, Katherine Maloney, Kayley. E Waltz, Chinmayee Rane, Sandeep Endluri, Phillip E. Savage*
4:24 Paper 8d: A Big Data Approach to Predict the Kinetics of Organic Chemistry Reactions — ***Stephanie Valleau***
4:42 Paper 8e: Uncertainty Quantification of Catalyst Structure Effects on Kinetics — ***Xue Zong***, *Dionisios Vlachos*
5:00 Paper 8f: Open Catalyst Project: Advancements and Challenges in Building a Flexible Machine Learning Potential — ***Muhammed Shuaibi***, *Lowik Chanussot, Siddharth Goyal, Thibaut Lavril, Abhishek Das, Morgane Riviere, Kevin Tran, Javier Heras-Domingo, Caleb Ho, Weihua Hu, Aini Palizhati, Anuroop Sriram, Brandon Wood, Junwoong Yoon, Devi Parikh, C. Lawrence Zitnick,* ***Zachary Ulissi***
5:18 Paper 8g: Machine Learning Accelerated Scale-up for Microporous Materials — ***Di Du***, *Anna Ivashko, Preeti Kamakoti, Stuart L. Soled*
5:36 Paper 8h: Physics-Informed Neural Networks for Kinetic Parameter Estimation and Uncertainty Quantification — ***Gabriel Gusmão***, *Adhika Retnanto, Shashwati da Cunha, Matthew Ross Kunz, Andrew Medford*

(9) Biocatalysis and Biobased Products

Sunday, Nov 7, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 110

Han Li, Chair
Jerome Fox, Co-Chair
Joshua Michener, Co-Chair

Sponsored by: Bioengineering

3:30 Paper 9a: Retrosynthesis Based on Chemical Similarity: Applications in Enzymatic Synthesis — ***Karthik Sankaranarayanan***, *Esther Heid, Connor Coley, Deeptak Verma, William Green, Klavs F. Jensen*
3:48 Paper 9b: Design Principles of Compartmentalization for Engineering Enzymatic Reactions — ***Dongheon Lee***, *Lingchong You*
4:06 Paper 9c: Asymmetric Catalysis with Artificial Metalloenzymes Based on dsDNA-Amphiphiles — ***Danyu Wang***, *Jun Guo, Huihui Kuang, Michael Tsapatsis, Efrosini Kokkoli*

4:24 Paper 9d: Accelerating the Discovery of Novel Ribosomally Synthesized and Post-Translationally Modified Peptides (RiPPs) through Pathway Refactoring and Robotic Automation — ***Chengyou Shi***, *Wilfred A. van der Donk, Douglas A. Mitchell, Huimin Zhao*
4:42 Paper 9e: Facile Fabrication of Antibacterial and Antiviral Perhydrolase-Containing Polymeric Composite Coatings — ***Shirley Xu***, *Li-Sheng Wang, Sneha Gopal, Matthew Brier, Jonathan S. Dordick*
5:00 Paper 9f: Rational Engineering of Cellulase Enzymes for Improved Biomass Conversion Via Reduced Non-Productive Binding — ***Bhargava Nemmaru***, *John Yarbrough, Madeline Johnson, Matthew J. Lang, Shishir Chundawat*
5:18 Paper 9g: Biosynthesis of Unusual Functionalities in Natural Products— ***Wenjun Zhang***

(10) Biomaterials: Faculty Candidates I

Sunday, Nov 7, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 103

Whitney Stoppel, Chair
Bret Ulery, Co-Chair
Ryan Koppes, Co-Chair
Iman Noshadi, Co-Chair

Sponsored by: Biomaterials

3:30 Paper 10a: Biomimetic Scaffolds Recapitulate Immune Cell Anti-Tumor Phenotypes in the Early Breast Cancer Metastatic Niche — ***Sophia Orbach***, *Michael Brooks, Scott Campit, Ryan Rebernick, Grace Bushnell, Sriram Chandrasekaran, Max Wicha, Jacqueline Jeruss, Lonnie Shea*
3:48 Paper 10b: Materials Approaches to Immune Engineering for Cancer and Autoimmune Diseases — ***Apoorv Shanker***
4:06 Paper 10c: Altering Vaccine Placement of Cytotoxic and Helper T Cell Antigens Influences Immunological Activation — ***Michelle Teplensky***, *Michael Evangelopoulos, Chad A. Mirkin*
4:24 Paper 10d: Nanoparticle-Augmented CAR T Cells for Combined Ultrasound and Photoacoustic Image-Guided Cancer Immunotherapy— ***Jinhwan Kim***, *Kelsey P. Kubelick, Lena Gamboa Castro, Gabriel A. Kwong, Stanislav Y. Emelianov*
4:42: Break
5:00 Paper 10f: Exploiting Nano-Bio Interface to Overcome Circulatory Barriers and Augment Vascular Theranostics — ***Kenry .***
5:18 Paper 10g: A Rapid Screening Platform for Protein Expression to Enable Materials Development — ***Melody Morris***, *Rogerio Bataglioli, Danielle Mai, Yun Jung Yang, Justin M. Paloni, Carolyn E. Mills, Zachary Schmitz, Erika A. Ding, Allison C. Huske, Bradley Olsen*
5:36 Paper 10h: High Fidelity Protein Interaction Prediction with Applications in Novel Biomaterials — ***Ratul Chowdhury***

(11) Carbon, Coal and Biomass Management

Sunday, Nov 7, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 300

David Lyons, Chair
Changle Jiang, Co-Chair

Sponsored by: Process Intensification & Microprocess Engineering

3:30 Paper 11a: Effect of Pyrolysis Conditions on Producing Mesophase Pitch from Varying Ranks of Coal and Correlating Their Product Properties with Machine Learning Models — ***Joshua Malzahn***, *Madison Cooley, Shikai Fang, Sudhanshu Sane, Shandian Zhe, Robert M. Kirby, Eric Eddings*
3:55 Paper 11b: Mild Solvolysis Liquefaction of Low-Rank Coal into a Feedstock of Value-Added Carbon Materials — ***Wenjia Wang***, *Ignacio Preciado, Joshua Malzahn, Eric Eddings*
4:20 Paper 11c: Modular Processing of Flare Gas for Carbon Nanoproducts— ***Jessica Hauck***, *Kent J. Warren, Gage Sowell, Mija H. Hubler, Theodore Champ, Andrew Broerman, Linfei Li, Boning Wang, Robert L. Anderson, Alan Weimer*

(12) CO_2 Upgrading: Photo/Reduction, Hydrogenation, and Thermal Upgrading

Sunday, Nov 7, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 206

Marc Porosoff, Chair
Madelyn R. Ball, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

3:30 Paper 12a: Selective Hydrogenation of CO_2 and CO over Potassium Promoted Co/ZSM-5 — ***Renjie Liu***, *Marc Porosoff*
3:48 Paper 12c: Enhancing Methanol Yield of CO_2 Hydrogenation with the Use of Bifunctional Catalyst/Adsorbent Formulations — ***Ting Lin***, *Aditya Bhan*
4:06 Paper 12d: The Influence of Plasma-Induced Surface Charging on Single-Atom Catalysis for CO_2 Reduction — ***Frank Doherty***, *Bryan Goldsmith*
4:24 Paper 12e: Plasmon-Induced CO_2 Conversion on Al@Cu_2O: A DFT Study— ***Tien Le***, *Yihan Shao, Bin Wang*
4:42 Paper 12f: CO_2 Hydrogenation over Mechano-Chemically Prepared Transition Metal-Based Ceria Catalysts — ***Juan Jimenez***, *Maila Danielis, Luis E. Betancourt, Sara Colussi, Alessandro Trovarelli, Jose A. Rodriguez, Sanjaya D. Senanayake*
5:00 Paper 12g: Materials Exhibiting Biomimetic Carbon Fixation and Self-Repair: A Mathematical Analysis of Carbon Fixing Materials — ***Dorsa Parviz***, *Daniel James Lundberg, Michael S. Strano*
5:18 Paper 124g: Feasibility Study of Combining Direct Air Capture of CO_2 and Methanation with Dual Function Materials (DFM) — ***Chae Jeong-Potter***, *Monica Abdallah, Robert Farrauto*

(13) Developments in Electrochemical Reactors, Fuel Cells, and Electrolyzers

Sunday, Nov 7, 3:30 PM
Marriott Copley Place, Fairfield

Jamelyn Holladay, Chair

Sponsored by: Fuels and Petrochemicals Division

3:30: Welcoming Remarks
3:35 Paper 13a: Caustic Aqueous Phase Ethanol Reforming for Process-Intensified Hydrogen Production — ***Benjamin Kee***, *Wei Jyun Wang, Martinus Dewa, James Seaba, Osman Akpolat, Patrick Littlewood, Su Ha*
3:55: Break
4:15: Break
4:35 Paper 13d: Spatiotemporal Decoupling of Cerium-Mediated Water Electrolysis for Grid Energy Storage and Hydrogen Generation — ***Daniel Frey***, *Ju hee Shin, Miguel Modestino*
4:55: Concluding Remarks

(14) Distributed Chemical and Energy Processes for Sustainability

Sunday, Nov 7, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 313

Shweta Singh, Chair
Carole Read, Co-Chair
Nick AuYeung, Co-Chair
Wenzhen Li, Co-Chair

Sponsored by: Sustainable Energy

3:30 Paper 14a: Local Renewable Chemical Production for Combined Heat and Power in Remote Locations: Optimal Design and Operation — ***Matthew Palys***, *Michael Reese, Prodromos Daoutidis*
3:45 Paper 14b: Distributed and on-Demand Ammonia Synthesis By Inorganic Membrane Reactor — ***Simona Liguori***
4:00 Paper 14c: Spatial Variation in Cost of Renewable Electricity-Driven Continuous Ammonia Production across the United States — ***Dharik Mallapragada***, *Nikifar Lazouski, Karthish Manthiram, Abhishek Bose, Michal Gala*
4:15 Paper 14d: Paired Electrolysis of Furanic Compounds to Valuable Chemicals in Electrochemical Flow Cells — ***Hengzhou Liu***, *Ting-Han Lee, Yifu Chen, Eric W. Cochran, Wenzhen Li*
4:30 Paper 14e: An Integrated Reaction and Separation Process for "Green Ammonia" Production from Distributed and Intermittent Renewable Energy.— ***Collin Smith***

(15) Electrocatalysis and Photoelectrocatalysis I: Photocatalysis and Oxygen Electrocatalysis

Sunday, Nov 7, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 203

Astrid M. Mueller, Chair
Robert Warburton, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

3:30: Break
3:48 Paper 15d: Optimizing Nanoscale Catalyst/Semiconductor Photoelectrocatalysts with Interfacial Design — ***Aarti Mathur***, *John Hemmerling, Suljo Linic*
4:06 Paper 15e: Theoretical Insight into Photo-Catalytic Pfas Degradation Mechanisms over Boron Nitride — *Yu Chen, Manav Bhati,* ***Thomas Senftle***
4:24 Paper 15f: *Mechanistic Insight into Water Oxidation to Ozone on Rutile Sno_2 (110) with Computational Chemistry* — ***Lingyan Zhao***, *Maureen Tang, John Keith*
4:42 Paper 15g: Systematic Tuning of Iridate Perovskite Catalysts to Probe Reaction and Degradation Mechanisms for Water Oxidation in Acidic Conditions— ***Linsey Seitz***
5:00 Paper 15h: Tailoring the Electronic Structure of Metal Cationic Centers in Non-Stoichiometric Mixed Metal Oxides for Enhanced Electrochemical Performance — ***John Carl A. Camayang***, *Samji Samira, Xiang-Kui Gu, Eranda Nikolla*

(16) Estimation and Control under uncertainty

Sunday, Nov 7, 3:30 PM
Sheraton Back Bay, Back Bay Ballroom D

Manjiri Moharir, Chair
Maria Papathanasiou, Co-Chair

Sponsored by: Systems and Process Control

3:30 Paper 16a: Dynamic Discrepancy Reduced-Order Modeling and Advanced Control of a Fischer-Tropsch Slurry Bubble Column Reactor — ***San Dinh***, *Jose Bohorquez, David S. Mebane, Fernando V. Lima*
3:49 Paper 16b: The Inherent Robustness of Model Predictive Control: Discrete and Infrequent Disturbances — ***Robert McAllister***, *James Rawlings*
4:08 Paper 16c: Fault Detection in Uncertain Nonlinear Chemical Systems: A Comparison of Advanced Set-Based Methods with Conventional Data-Driven and Observer-Based Methods — ***Bowen Mu***, *Xuejiao Yang, Joseph K. Scott*
4:27 Paper 16d: Data-Driven Online Scenario Selection for Multistage NMPC— ***Zawadi Mdoe***, *Mandar Thombre, Johannes Jäschke*
4:46 Paper 16e: State Observer Design and Model Predictive Control of an Industrial-Scale Biochemical Fermenter — ***Parth Shah, Masters***, *M. Ziyan Sheriff, Mohammed Saad Faizan Bangi, Joseph Kwon, Costas Kravaris*
5:05 Paper 16f: Robust Model Predictive Control for Large-Scale Distributed Parameter Systems Under Uncertainty — ***Min Tao***, *Constantinos Theodoropoulos*

5:24 Paper 16g: Stochastic Optimal Control of Polynomial Jump-Diffusion Processes Via Local Occupation Measures — ***Flemming Holtorf***, *Paul I. Barton*
5:43 Paper 16h: Optimal Control of Dose Delivery in Atmospheric Pressure Plasma Jets — ***Diogo Rodrigues***, *Kimberly Chan, Ali Mesbah*

(17) Experimental and Computational Approaches to Accelerate and Discover Inorganic Materials

Sunday, Nov 7, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 101

Peng Bai, Chair
Satish Nune, Co-Chair

Sponsored by: Inorganic Materials

3:30 Paper 17e: Electron Beam Induced Modification of ZIF-8 Membrane Permeation Properties — ***Yurun Miao***, *Dennis Lee, Michael Tsapatsis*
3:50 Paper 17b: Solid-State Synthesis Planning for Inorganic Materials— ***Joseph Montoya***, *Muratahan Aykol*
4:10 Paper 17c: A Recommendation System to Predict Missing Adsorption Properties of Nanoporous Materials — *Arni Sturluson, Ali Raza, Grant McConachie, Daniel Siderius, Xiaoli Fern,* ***Cory Simon***
4:30 Paper 17d: Comprehensive Study of Surface Segregation across Ternary Alloy Composition Space: Cuauag — ***Zhitao Guo***, *Andrew J. Gellman*

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

Sunday, Nov 7, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 308

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

Sponsored by: Fundamentals

3:30 Paper 18a: An Optimization Framework for the Evaluation of Energy-Water Systems for Agricultural Applications — ***Marcello Di Martino***, *Sarah Namany, Styliani Avraamidou, Tareq Al-Ansari, Efstratios N. Pistikopoulos*
3:45 Paper 18b: Practical Considerations of a Moringa Seed Coated Filter for Water Purification — ***Stephanie Velegol***, *Laxmicharan Samineni, Manish Kumar*
4:00 Paper 18c: Fully Functional Large-Area Nanoporous Single Layer Graphene Membranes for Desalination and Water Purification — ***Piran Kidambi***
4:15 Paper 18d: The Investigation of Industrial Crop Production in Arid Regions— ***Sarah Alnouri***, *Nivinya Hemachandra, Beena Debnath, Vishmi Singhapura, Nafia Tasneem, Hiba Namany, Dhabia Al-Mohannadi, Debalina Sengupta*

(19) Fundamentals of Interfacial Phenomena I

Sunday, Nov 7, 3:30 PM
Sheraton Back Bay, Back Bay Ballroom B

Sujit Datta, Chair
Dongjin Seo, Co-Chair
Sepideh Razavi, Co-Chair

Sponsored by: Interfacial Phenomena

3:30 Paper 19a: Theory of Overscreening at Charged Surfaces — ***Pedro de Souza***, *Martin Z. Bazant*
3:45 Paper 19b: Hidden Ion Structures and Underscreening in Concentrated Electrolytes — ***Emily Krucker-Velasquez***, *James Swan*
4:00 Paper 19c: Diffusiophoresis in Microfluidic Dead-End Configuration: Influence of the Environment — ***Suin Shim***, *Ankur Gupta, Benjamin M. Alessio, Jessica Wilson, Luqman Issah, Emmanuel Mintah, Yingxian E. Yu, Howard A. Stone*
4:15 Paper 19e: Automated Langmuir-Blodgett Deposition of Particles on a Non-Flat Surface — ***Samuel Wilson-Whitford***, *Midhun Joy, Xue Li, Maria Chiara Roffin, James Gilchrist*
4:30 Paper 19f: Visualizing Drying Stresses in Liquid Coatings on Soft Substrates — ***Shashank Kamdar***, *Xiang Cheng, Lorraine F. Francis*
4:45 Paper 19g: Influence of Interfacial Rheology on Viscous Fingering — ***Jiayu Li***, *Harishankar Manikantan*
5:00 Paper 19i: Characterizing the Hydrophobic Interactions of Fusion Peptides of Coronaviruses Using Single-Molecule Force Measurements — ***Cindy Qiu***, *Miya K. Bidon, Susan Daniel, Nicholas L. Abbott*
5:15 Paper 19j: Effect of Cyclodextrins on Fluorinated Surfactant Micelles — *Samhitha Kancharla, Yuxin Bao, Paschalis Alexandridis,* ***Marina Tsianou***

(20) Green Chemical Reaction Engineering for Sustainability

Sunday, Nov 7, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 205

Hsu Chiang, Chair
Wan-Ting Chen, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

3:30: Break
3:50: Break
4:10 Paper 20c: Discriminating between Energy Sources for Chemical Reactions — ***Zachary Schiffer***, *Aditya Limaye, Karthish Manthiram*
4:30 Paper 159as: Sustainable Production of Protein and Fiber Concentrates from Defatted Soybean Flour By Tribo-Electrostatic Separation — ***Botagoz Kuspangaliyeva***, *Dinara Konakbayeva, Solmaz Tabtabaei*
4:50 Paper 20e: Solvent Optimization for Extraction of High Commercial Value Chemicals from Food Waste — ***Yagya Gupta***, *Souryadeep Bhattacharyya, Dionisios Vlachos*
5:10 Paper 20f: Cost and Energy Efficient Cyclic Separation of 5-Hydroxymethyl Furfural from an Aqueous Solution — ***Yung Wei Hsiao***, *Aikaterini Anastasopoulou, Marianthi Ierapetritou, Dionisios Vlachos*
5:30 Paper 20g: Enhanced Hydrogenation of Oleic Acid By RF Heating Via Magnetically Susceptible Nanoparticles — ***Cameron Roman***, *Natalia da Silva Moura, Scott Wicker, Kerry M. Dooley, James Dorman*

(21) Industry 4.0, Digital Twins, and Digital Transformation I

Sunday, Nov 7, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 201

Akhilesh Jain, Chair
Heleno Bispo, Co-Chair

Sponsored by: Next-Gen Manufacturing

3:30 Paper 21a: Accelerating Time to Competency in an Industry 5.0 World— ***Ian Willetts***, ***Brent Kedzierski***
3:53 Paper 21b: How to Get a Head Start on Your Digitalization Journey— ***Jonas Norinder***
4:16 Paper 21c: Development of an Advanced Control Infrastructure for Subcritical Power Plant Online Power Demand Tracking — ***Daniel Kestering***, *Selorme Agbleze, David Tucker, Lawrence J. Shadle, Heleno Bispo, Fernando V. Lima*
4:39 Paper 21d: CFD Based Study to Predict Rollover in an Industrial LNG Storage Tank — ***Suraj Prakash Singh***, ***Rajagopalan Srinivasan***, ***Iftekhar Karimi***
5:02 Paper 21e: Digital Twin of Renewable Energy-Linked Power-to-Gas (P2G) Systems: Model Building and Continuous Update for Hydrogen Producing Electrolysis — ***Yongbeom Shin***, *En Sup Yoon, Dongil Peter Shin*
5:25 Paper 21f: Keynote Talk - Artificial Intelligence and the Modern Workforce— ***Philippe Herve***

(23) Life Cycle Analysis of Bio-Based Fuels, Energy, and Chemicals

Sunday, Nov 7, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 311

David Shonnard, Chair
Yuan Yao, Co-Chair

Sponsored by: Sustainable Biorefineries

3:30 Paper 23a: Life Cycle GHG Emissions, Water and Fossil-Fuel Consumption for Polyethylene Furanoate (PEF) and Its Co-Products from Lignocellulosic Biomass *Via* Furanics Conversion — ***Taemin Kim***, *Pahola Thathiana Benavides, Ulises R. Gracida-Alvarez, James Bamford*
3:45 Paper 23b: Techno-Economic Greenhouse Gas Life Cycle Assessment of the CO_2-EOR Operations on Farnsworth Unit — ***Anthony Morgan***, *Reid Grigg, William Ampomah*
4:00 Paper 23c: Life Cycle Analysis and Techno-Economic Assessment of Emerging Sustainable Polymer Processes — ***Sabyasachi Das***, *Jennifer B. Dunn*
4:15 Paper 23d: Carbon Footprint and Land Use Reductions of Electromicrobial Production Systems Quantified By Process Modelling and Comparative Life Cycle Assessment — ***Jeremy Adams***, *Anthony Abel, Douglas S. Clark*
4:30 Paper 23e: Integrated Biorefinery Design Under Multi-Scale Uncertainties— ***Yuqing Luo***, *Marianthi Ierapetritou*

(24) Lignin for Sustainable Industrial Uses

Thursday, Nov 18, 12:30 PM
Virtual, Forest and Plant Bioproducts Division (17)

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

Sponsored by: Forest and Plant Bioproducts Division

12:30 Paper 24a: Activated Carbon from High-Purity Lignin with Controlled Molecular Weight — ***Chengjun Wu***, *Graham Tindall, Junhuan Ding, Zachariah Pittman, Mark Thies, Mark E. Roberts*
12:50 Paper 24b: Production of High-Quality Carbon Fiber from Lignin Precursor — *Yixin Luo,* ***Xianglan Bai***
1:10 Paper 24c: Exploiting the Liquid-Liquid Phase Behavior of Hybrid Poplar Lignin in Ethanol-Water Solutions to Produce Precursors for Value-Added Applications — ***Graham Tindall***, *Bronson Lynn, Villő E. Bécsy-Jakab, Mark Thies, David Hodge*
1:30 Paper 24d: Synthesis of Charged Lignin Nanoparticles and Its Applications As Adsorbent — ***Mandeep Poonia***, *Kwang Ho Kim, Xianzhi Meng, Udani Kaushalya Wijethunga, Arthur J. Ragauskas, Gyu Leem, Chang Geun Yoo*
1:50 Paper 24e: Techno-Economic Analysis and Life Cycle Assessment of Lignin Fractionation and Valorization Via the ALPHA Process: Upgrading to Value-Added Products — ***Daniel Kulas***, *Mark Thies, David Shonnard*

(25) Mechanical Cues and Cell Behavior

Sunday, Nov 7, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 108

Panagiotis Mistriotis, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

3:30 Paper 25a: Exploring Interactions between Primary Hepatocytes and Non-Parenchymal Cells on Physiological and Pathological Liver Stiffness — ***Youra Moeun***, *Vaishaali Natarajan, Srivatsan Kidambi*
3:48 Paper 25b: Expression of Glycocalyx on Human Lung Microvascular Endothelial Cells Is Shear Stress and Time Dependent — ***Natasha Cruz-Calderon***, *Camden Holm*

4:06 Paper 25c: The Fluid Shear Stress Sensor TRPM7 Regulates Cell Intravasation — ***Kaustav Bera***, *Christopher L. Yankaskas, Konstantin Stoletov, Selma Serra, Julia Carrillo-Garcia, Soontorn Tuntithavornwat, Panagiotis Mistriotis, John Lewis, Miguel Valverde, Konstantinos Konstantopoulos*
4:24 Paper 25d: Effects of Fluid Shear Stress on Reactive Oxygen Species Generation, Stemness, and Epithelial-to-Mesenchymal Transition — ***Spenser Brown***, *Juliana Bates, Alexandra Avera, Yonghyun Kim*
4:42 Paper 25e: Shear Stress in a Spinner Flask Bioreactor Alters Energy Metabolism and Replicative Senescence of Human Mesenchymal Stem Cells— ***Richard Jeske***, *Chang Liu, Xingchi Chen, Laurie Muok, Xuegang Yuan, Yan Li*
5:00 Paper 25h: Mechanotransduction during Confined Cell Migration— ***Panagiotis Mistriotis***
5:18 Paper 25g: Mechanical Cues and Cell Behavior – Immune, Stem, and Tumor Cell Examples (Invited Speaker) — ***Dennis E. Discher***

(26) Microfluidic and Millifluidic Techniques to Study Nanoscale Materials

Thursday, Nov 18, 12:30 PM
Virtual, Nanoscale Science and Engineering Forum (22)

Steven Saunders, Chair

Sponsored by: Nanoscale Science and Engineering Forum

12:30 Paper 26a: Probing Topological Transitions of Inverse Worm-like Micelles Subject to Transient Shear Flow Using Dielectric Spectroscopy and Neutron Scattering — *Noah Cho, John Riley,* ***Jeffrey Richards***
12:55 Paper 26b: Optimized Continuous Millifluidic Surface Modification of Synthesized Silver Nanowires with Palladium — ***Destiny Williams***, *Shohreh Hemmati, James Smay*
1:20 Paper 26c: Application of a Continuous Flow Millifluidic Reactor Towards Optimizing Manufacturing Throughput for Molybdenum Carbide Nanoparticles— ***Majed Madani***, *Lanja R. Karadaghi, Emily M. Williamson, Susan E. Habas, Frederick Baddour, Richard L. Brutchey, Noah Malmstadt*
1:45: Break

(27) Multiphase & Liquid Phase Reaction Engineering

Tuesday, Nov 9, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 208

Joris Thybaut, Chair
Sankar Dinesh Kumar Kalaga, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

12:30 Paper 27a: Intensified Production of Renewable Fuels and Chemicals: Rational Design of Heterogeneous Aminated Catalysts for Liquid Phase Aldol Reactions — ***Jeroen Lauwaert***
12:54 Paper 27b: Synthesis of Fatty Amines: Rhodium-Catalyzed One-Pot Hydroaminomethylation of 1-Decene in an Aqueous Multiphase System— ***Ariane Weber***, *Reinhard Schomaecker*
1:12 Paper 27c: Multiscale Modelling of Biomass Fast Pyrolysis in Micro Fluidized Beds — ***Balivada Kusum Kumar***, *Subhajit Dutta, Himanshu Goyal*
1:30 Paper 27d: Multiphase Operations in the Taylor-Couette Disc Contactor— ***Georg Rudelstorfer***, *Susanne Lux, Matthaeus Siebenhofer, Annika Grafschafter*
1:48: Break
2:06: Break
2:24 Paper 27h: Nucleophilic Aromatic Substitution in High-Temperature Ionic Liquids — ***Azin Eftekhari***, *Edward Anderson, James H. Davis Jr., Kevin West, Brooks D. Rabideau, Christy West*

(28) Nanobiotechnology for Sensors and Imaging

Sunday, Nov 7, 3:30 PM
Marriott Copley Place, Simmons

Daniel Roxbury, Co-Chair
Nigel Reuel, Co-Chair

Sponsored by: Bionanotechnology

3:30 Paper 28a: Graduate Student Award Session: Development of Stable Targeted Nano-, Encapsulated Manganese Oxide (NEMO) Particles for Early Breast Cancer Diagnosis By MRI — ***Celia Martinez de la Torre***, *Kasey Freshwater, Margaret Bennewitz*
3:50 Paper 28c: Multispectral Fingerprinting Resolves Dynamics of Nanomaterial Trafficking in Primary Endothelial Cells — ***Mitchell Gravely***, *Daniel Roxbury*
4:10 Paper 28d: Continuous Free-Flow Isoelectric Separation of Extracellular RNA Nanocarriers from Plasma — ***Himani Sharma***, *Satyajyoti Senapati, Hsueh-Chia Chang*
4:30 Paper 28e: Superparamagnetic Nanobead and Electrodeposited Magnetic Nanoporous Membrane for Immunocapture of Specific Exosomes— ***Chenguang Zhang***, *Xiaoye Huo, Ceming Wang, Satyajyoti Senapati, Hsueh-Chia Chang*
4:50 Paper 28f: Dynamics Monitoring of Temozolomide and 5-Aminoimidazole-4-Carboxamide for Glioblastoma Using Fluorescent Nanosensors — ***Manki Son***, *Freddy T. Nguyen, Punit Mehra, Michael A. Lee, Naveed Bakh, Xun Gong, Xiaojia Jin, Volodymyr Koman, Michael S. Strano*
5:10 Paper 28g: Nanoparticles in Circulating Tumor Cells (CTC) — ***Suresh Ahuja***
5:30 Paper 28h: Gold Nanorod-Melanin Hybrids for Enhanced and Prolonged Photoacoustic Imaging in the Near-Infrared-II Window — ***Wonjun Yim***, *Jiajing Zhou, Jesse Jokerst*

(29) Operation of Energy Systems

Sunday, Nov 7, 3:30 PM
Sheraton Back Bay, Independence Ballroom East

Jianping Li, Co-Chair
Michael Short, Co-Chair
Xiaonan Wang, Co-Chair

Sponsored by: Systems and Process Operations

3:30 Paper 29a: Dynamic Modeling and Application of Model Predictive Control to the Cool-Down Process of a Liquefied Natural Gas (LNG) Tank— ***Kyeongseok Shin***, *Sang Hwan Son, Sungwon Hwang, Joseph Kwon*
3:49 Paper 29b: Renewables-Assisted Flexible Carbon Capture: A Dynamic Optimization Framework for Transitioning Towards Clean Energy — ***Manali S. Zantye***, *Akhil Arora, M M Faruque Hasan*
4:08 Paper 29c: Integrating Energy Storage in Power Production: A Design and Scheduling Approach — ***Antonio Sánchez***, *Qi Zhang, Mariano Martin, Pastora Vega*
4:27 Paper 29d: Integration Opportunities for Liquid Air Energy Storage— ***Zhongxuan Liu***, *Truls Gundersen*
4:46 Paper 29e: A Multi-Scale Modeling Paradigm for Energy System Operation and Design — *Xian Gao,* ***Alexander Dowling***
5:05 Paper 29f: A New Approach for Optimization of Detailed Shell-and-Tube Heat Exchanger Designs for Multi-Period Operation — *Zain Mahmoud, Ishanki De Mel, Saif Kazi,* ***Michael Short***
5:24 Paper 29g: Condition-Based Maintenance Scheduling and Planning for Multi-Component Energy Systems — ***Yaqing Wu***, *Christos Maravelias*
5:43 Paper 29h: Conceptual Design Via Superstructure Optimization in Advanced Energy Systems Using Idaes — ***Edna Rawlings***, *Naresh Susarla, Jaffer Ghouse, Miguel A. Zamarripa, Carl D. Laird, John Siirola, Michael Bynum, David Miller*

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

Friday, Nov 19, 3:30 PM
Virtual, Process Development Division (12)

Kishori Deshpande, Chair

Sponsored by: Product Design

3:30 Paper : Panel Discussion: Chemical Process and Product Design Careers in Industry & Academia — ***Kishori Deshpande***, ***Jim Pfaendtner***, ***Aditi Deshpande***, ***Jennifer L. Anthony***

(31) Polymer Crystallization and Semi-Crystalline Polymers

Sunday, Nov 7, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 105

Julie Albert, Chair
Jay Park, Co-Chair

Sponsored by: Polymers

3:30 Paper 31a: Controlling Stress Relaxation, Deformation, and Crystallinity in Semi-Crystalline Networks Using Dynamic Covalent Bonds — ***Alexa Kuenstler***, *Christopher Bowman*
3:45 Paper 31b: Molecular Dynamics Simulations of the Crystallization of Polyethylene As a Function of Chain Orientation — ***Ronald Larson***, *Wenlin Zhang, Yanan Gong*
4:15 Paper 31c: Free Energy Surfaces for Homogeneous Nucleation in a Polymer Melt — ***Douglas Tree***, *Pierre Kawak, Dakota S. Banks*
4:30: Break
4:45 Paper 31e: Molecular Dynamics Simulations of Crystal Nucleation in Incompatible Polymer Blends — ***Wenlin Zhang***
5:00 Paper 31f: A Thermodynamically Inspired Method for Quantifying Phase Transitions in Polymeric Liquids with Application to Flow-Induced Crystallization of a Polyethylene Melt — ***Mohammad Hadi Nafar Sefiddashti***, *Brian J Edwards, Bamin Khomami*
5:15 Paper 31g: Short-Chain Branching and Rheology of Crystallizing LLDPEs— ***Marat Andreev***, *Gregory Rutledge, Anthony Kotula, Jonathan Moore, Jaap den Doelder*
5:30 Paper 31h: Flow-Induced Crystallization of a Polyethylene Liquid Above the Melting Temperature and Its Nonequilibrium Phase Diagram — *Mohammad Hadi Nafar Sefiddashti, Brian J Edwards,* ***Bamin Khomami***
5:45 Paper 31i: Melting Kinetics, Ultra-Drawability and Microstructure of Nascent Ultra-High Molecular Weight Polyethylene Powder — ***Fotios Christakopoulos***, *Enrico M. Troisi, Alla S. Sologubenko, Nicolaas Friederichs, Laura Stricker, Theo A. Tervoort*

(32) Polymer Networks and Gels

Sunday, Nov 7, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 104

Nese Orbey, Chair
Monirosadat Sadati, Co-Chair
Jinhye Bae, Co-Chair

Sponsored by: Polymers

3:30 Paper 32a: Dual-Responsive Microgels for Morphological and Functional Repair of Nonwovens — ***Srivatsan Ramesh***, *Jack Davis, Alexandra Roros, Justin Eiben, Thomas Fabiani, Ryan Smith, Lewis Reynolds, Benham Pourdeyhimi, Saad A. Khan, Jan Genzer, Stefano Menegatti*
3:45 Paper 32b: Flexible Towel-like Polymer That Can Rapidly Mop up Blood— ***Hema Choudhary***, *Matthew B. Dowling, Srinivasa R. Raghavan*
4:00: Break
4:15: Break
4:30 Paper 32g: Fracture in Polymer Networks with Topological Defects— ***Bradley Olsen***, *Akash Arora, Tzyy-Shyang Lin, Haley Beech, Hidenobu Mochigase, Rui Wang*
5:00 Paper 32h: Fabrication and Characterization of Lignin-Based, Thermo-Responsive Soft Composite Materials — ***Missoury Lytle***, *Emily Miller, Katarina Keppler, Graham Tindall, Mark Thies, Eric M. Davis*

5:15 Paper 32i: Role of Chain Walking and Hopping on Anomalous Self-Diffusion in Linear Associative Polymer Gels — ***Ameya Rao***, *Jorge Ramirez, Bradley Olsen*
5:30 Paper 32d: How Carboranes Provide Tremendous Improvement in Thermal Stability of Thermosets for Aerospace and Defense Applications?— ***Shailja Goyal***, *Michael J. Forrester, Scott Carnahan, Sabrina Torres, Danielle Coverdell, Mark W. Lee Jr., Aaron Rossini, Eric W. Cochran*
5:45 Paper 32c: Reprocessable Polyhydroxyurethane Networks Reinforced with Polyhedral Oligomeric Silsesquioxanes (POSS) — ***Sumeng Hu***, *Xi Chen, John Torkelson*

(33) Polymer Viscoelasticity: Mechanics, Processing, and Rheology

Sunday, Nov 7, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 102

Ralm Ricarte, Chair
Vivek Sharma, Co-Chair
Sara Hashmi, Co-Chair
Jeff Ting, Co-Chair

Sponsored by: Polymers

3:30 Paper 33a: Mitigation of Hysteresis in High Solids Content Polymers Using Photorheometry — ***John Reynolds***, *Daniel Rau, Jackson Bryant, Christopher B. Williams, Michael Bortner*
3:45 Paper 33b: A Combined Torsional-Axial DMA Platform for Determination of Viscoelastic Poisson's Ratio — ***Abhishek Shetty***
4:00 Paper 33c: Towards Rheological Structure-Property Relationships: New Material Functions Based on Recoverable Strain, & Frequency-Sweep Medium-Amplitude Oscillatory Shear (MAOS) — ***Piyush Singh***, *Randy H. Ewoldt, Simon Rogers*
4:15 Paper 33d: Tying Formulation and Extensional Rheology to Processability in the Manufacturing of Ultrafine Fibers Via Electrospinning — *Elena Ewaldz, Joshua Randrup,* ***Blair Brettmann***
4:45: Break
5:00 Paper 33f: Pinching Dynamics, Rheology and Elastic Instabilities of Boger Fluids — ***Alexander Kubinski***, *Fahed Albreiki, Vivek Sharma*
5:15 Paper 33i: Polysaccharides As Food Thickeners — ***Karthika Suresh***, *Leidy N. Jimenez, Chenxian Xu, Lena Hassan, Stefan Baier, Vivek Sharma*
5:30 Paper 33g: Rheology and Pinching Dynamics of Associative Polysaccharide Solutions — ***Chenxian Xu***, *Jelena Dinic, Xinyu Lu, Chao Wang, Reza Rock, Hao Sun, Vivek Sharma*
5:45: Break

(34) Pyrolysis of Biomass

Sunday, Nov 7, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 207

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

Sponsored by: Catalysis and Reaction Engineering Division

3:30 Paper 34a: Experimental and Computational Insights into Secondary Decomposition Chemistry in Cellulose Pyrolysis — ***Pavlo Kostetskyy***, *Evan Terrell, Melba D. Denson, Manuel Garcia-Perez, Linda Broadbelt*
3:45 Paper 34b: Elucidating Lignin Pyrolysis Using Kmc Modeling — ***Maksim Tyufekchiev***, *Linda Broadbelt*
4:00: Break
4:15 Paper 34d: Energetics of Condensed-Phase Biomass Pyrolysis Chemistry: A Novel Computational Approach and Its Benchmarking Using *Ab-Initio*Molecular Dynamics — ***Arul Mozhi Devan Padmanathan***, *Samir H. Mushrif*

(35) Rational Design and Optimization of Soft Materials

Sunday, Nov 7, 3:30 PM
Marriott Copley Place, Salon A/B

Poornima Padmanabhan, Chair
Kathleen McEnnis, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

3:30 Paper 35a: Examining the Self-Assembly of Patchy Alkane-Grafted Silica Nanoparticles Using Molecular Simulation — ***Nicholas Craven***, *Justin Gilmer, Caroline J. Spindel, Andrew Z. Summers, Christopher Iacovella, Clare McCabe*
3:45 Paper 35b: Factors Influencing the Self-Assembly of Glycolipids into Three-Dimensional Network Phases — ***Ke Luo***, *Zhengyuan Shen, Mahesh Mahanthappa, Joern Siepmann*
4:00 Paper 35c: Hierarchical Self-Assembly Pathways of Peptoid Helical Rods and Sheets — ***Mingfei Zhao***, *Kacper Lachowski, Sarah Alamdari, Janani Sampath, Peng Mu, Lilo Pozzo, Chunlong Chen, Christopher J. Mundy, Jim Pfaendtner, Andrew Ferguson*
4:15 Paper 35d: Peptide Framework for Screening the Effects of Amino Acids on Assembly — ***Seren Hamsici***, *Andrew White, Handan Acar*
4:30 Paper 35e: Multi-State Monte Carlo Optimization of Electrostatic Domain Differences for Self-Assembling Proteins — ***Dustin Britton***, *Chengliang Liu, Michael Meleties, Sihan Jia, Kamia Punia, Jay Kang, Jin Kim Montclare*
4:45 Paper 35f: Directed Assembly and Motion of Patterns in Active Matter — *Caroline Desgranges,* ***Jerome Delhommelle***
5:00 Paper 35g: Crystal Structure Discovery through Interaction Potential Variation — ***Hillary Pan***, *Julia Dshemuchadse*
5:15 Paper 35h: Adaptive Mechanical Properties of Colloidal Crystals *Via* Active Interstitials — ***Bryan VanSaders***, *Sharon C. Glotzer*
5:30 Paper 35i: The Diversity of Three-Dimensional Photonic Crystals for Colloidal Self-Assembly — ***Rose Cersonsky***, *James Antonaglia, Bradley Dice, Sharon C. Glotzer*
5:45 Paper 35j: Anisotropic Nanocrystal Shape and Ligand Design for Co-Assembly — ***Thi Vo***, *Katherine Elbert, William Zygmunt, Corbin Vara, Daniel Rosen, Nadia M. Krook, Sharon Glotzer, Christopher B. Murray*

(36) Reactor Engineering for Biomass Feedstocks

Sunday, Nov 7, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 312

Christos Maravelias, Chair
Yukihiko Matsumura, Co-Chair

Sponsored by: Sustainable Biorefineries

3:30: Break
3:45 Paper 36b: A Model-Based Approach for the Shift from Batch to Continuous Production of Succinic Acid from Glycerol — ***Ioannis Zacharopoulos***, *Constantinos Theodoropoulos*
4:00 Paper 36c: Low Temperature Reactors for Biomass Processing and Carbon Modification Using Atmospheric Pressure Plasmas — ***David Barlaz***, *David Ruzic*
4:15 Paper 36d: Effect of Particle Size on Supercritical Water Gasification of Biomass — ***Yukihiko Matsumura***, *Bailun Chen, Yuki Koshiishi*
4:30 Paper 36e: Catalytic Deoxygenation of Rapeseed Oil into Drop-in Fuel Under Hydrothermal Condition Causing *in-Situ* Hydrogen Production — ***Masato Kouzu***, *Minato Kojima, Katsuyuki Mori, Haruka Ishida, Jun Suzuki*
4:45 Paper 36f: Ash Adhesion on Inconel Mesh during Bamboo Powder Combustion — ***Kenichiro Tanoue***, *Kazuma Takata, Nao Umehara, Morihisa Yokota, Toyoaki Niki*

(37) Retaining Women in Chemical Engineering Careers

Tuesday, Nov 16, 3:30 PM
Virtual, Engineering for Inclusion (TC)

Lisa Volpatti, Co-Chair
Quinta Nwanosike Warren, Co-Chair
Aditi Khadilkar, Co-Chair
Sarika Goel, Co-Chair

Sponsored by: Women in Chemical Engineering Committee (WIC)

3:30 Paper 37a: Retaining Women in Chemical Engineering Careers Panel Discussion — ***David Friedman***, ***Dennis Hess***, ***Helene Harding***, ***Meagan Lewis***, ***Debalina Sengupta***

(38) Self-Assembly in Solution

Sunday, Nov 7, 3:30 PM
Sheraton Back Bay, Back Bay Ballroom A

Paschalis Alexandridis, Chair
Yakov Lapitsky, Co-Chair
Javen Weston, Co-Chair

Sponsored by: Interfacial Phenomena

3:30 Paper 38a: Molecular Modeling of Self-Assembled Peptide-Based Nanoparticles — ***Shivangi Nangia***, *Irene Primo Calvo-Manzano, Denny Mathew*
3:45 Paper 38b: Structure Control of Arrested Bicontinuous Channels Via a New Type of Colloidal Gel — ***Yuyin Xi***, *Juscelino Leão, Qiang Ye, Ronald Lankone, Li-Piin Sung, Yun Liu*
4:00 Paper 38c: ROS-Induced Disruption of Vesicles: A Potential Strategy to Enhance Cancer Radiotherapy — ***Sai Nikhil Subraveti***, *Narottam Lamichhane, Srinivasa R. Raghavan*
4:15 Paper 38d: Molecular Self-Assembly in Nematic Solvents — ***Soumik Das***, *Junghyun Noh, Wei Cao, Hao Sun, Nathan Gianneschi, Nicholas L. Abbott*
4:30 Paper 38e: Structure and Composition of Mixed Micelles Formed By Ionic Surfactants and Nonionic Block Copolymers in Water — ***Samhitha Kancharla***, *Marina Tsianou, Paschalis Alexandridis*
4:45 Paper 38f: Liquid Crystalline Coacervates Composed of Chromonic Mesogens and Polyelectrolytes — ***Elizabeth Adeogun***, *Divya Iyer, Samanvaya Srivastava, Karthik Nayani*
5:00 Paper 38g: *High Performance Sulfate-Free Cleansers: Surface Activity, Foaming, and Rheology* — ***Kelly Yorke***, *Andrei Potanin, Suzanne Jogun, Andre Morgan, Hongwei Shen, Samiul Amin*
5:15 Paper 38h: Foam Film Stratification Studies Probe Intermicellar Interactions — *Chrystian Ochoa, Shang Gao, Samanvaya Srivastava,* ***Vivek Sharma***
5:30 Paper 38i: Equilibrium and Dynamic Surface Tension of per- and Polyfluoroalkyl Substances at Air-Water Interface — ***Zahra Abbasian Chaleshtari***, *Reza Foudazi*
5:45 Paper 38j: Constant Surface Area Surfactant Adsorption for Microtensiometers — ***Steven Iasella***, *Joseph Zasadzinski*

(39) Software Engineering in and for the Molecular Sciences

Sunday, Nov 7, 3:30 PM
Marriott Copley Place, Salon J/K

Eric Jankowski, Chair
Utkarsh Kapoor, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

3:30 Paper 39a: The Molecular Simulation Design Framework (MoSDeF) Project: A Collaboration Towards Transparent, Reproducible, Usable By Others, Extensible (TRUE) Simulations — ***Justin Gilmer***, *Co D. Quach, Ray Matsumoto, Parashara Shamaprasad, Ryan S. DeFever, Ramanish Singh, Brad Crawford, Eric Jankowski, Arthi Jayaraman, Jeremy Palmer, Edward J. Maginn, Joshua Anderson, Sharon C. Glotzer, Joern Siepmann, Jeffrey Potoff, Christopher Iacovella, Ákos Lédeczi, Clare McCabe, Peter Cummings*

3:46 Paper 39b: Testing and Validation of an Automated Iterative Boltzmann Inversion (IBI) Code — *Lilian Johnson, **Frederick Phelan Jr.***
4:00 Paper 39c: Screening of Organic Photovoltaic Morphologies Enabled By Mosdef Tools, Continuous Integration, and Test-Driven Development. — ***Jenny Fothergill**, Chris Jones, Matthew Jones, Michael Henry, Justin Gilmer, Ryan S. DeFever, Edward J. Maginn, Clare McCabe, Peter Cummings, Eric Jankowski*
4:16 Paper 39d: How a Quantum Computer Could Solve a Microkinetic Model— ***Eric Walker**, Shreyas Addamane Pallathadka, Anand Prabhu, Sri Charan Simha Velpur, Mary Sharmila Rongali*
4:32 Paper 39e: Performant Python Extensions in HOOMD-Blue Version 3.0— ***Brandon Butler**, Joshua Anderson, Sharon Glotzer*
4:48: Break
5:04 Paper 39g: GOMC-MoSDeF: A Module for Generating the Required Files for Conducting Monte Carlo Simulations via the GOMC and MoSDeF Software— ***Brad Crawford**, Jeffrey Potoff*
5:20 Paper 39h: Aiidalab, an Ecosystem for Developing, Executing, and Sharing Scientific Workflows — *Aliaksandr V. Yakutovich, Kristjan Eimre, Ole Schütt, Leopold Talirz, **Carl Simon Adorf**, Casper W. Andersen, Edward Ditler, Dou Du, Daniele Passerone, Berend Smit, Nicola Marzari, Giovanni Pizzi, Carlo A. Pignedoli*
5:36 Paper 39i: Signac: Data Management and Workflows for the Molecular Sciences — ***Brandon Butler**, Bradley Dice, Sharon C. Glotzer*

(40) Software Tools and Implementations for Process Systems Engineering

Sunday, Nov 7, 3:30 PM
Sheraton Back Bay, Back Bay Ballroom C

Ruth Misener, Chair
Ali Mesbah, Co-Chair
Kristen Severson, Co-Chair

Sponsored by: Computing Systems and Technology Division

3:30 Paper 40a: Romodel: Modelling Robust Optimization Problems in Pyomo— *Johannes Wiebe, **Ruth Misener***
3:45 Paper 40b: New Features and Comprehensive Benchmarking Study of the Pyomo Robust Optimization Solver — ***Natalie Isenberg**, Chrysanthos Gounaris, John Siirola*
4:00 Paper 40c: Ppopt (Python Parametric OPTimization) - a Python Package for Solving Multiparametric Optimization Problems with Parallel Algorithms— ***Dustin Kenefake**, Efstratios N. Pistikopoulos*
4:15 Paper 40d: Parapint: Scalable Parallel Solution of Structured Nonlinear Programs — *Michael Bynum, Jose Rodriguez, **Carl D. Laird**, Bethany Nicholson, Jordan Jalving, John Siirola, Denis Ridzal*
4:30 Paper 40e: Diagnostic Tools for Nonlinear Algebraic Models of Dynamic Chemical Processes in Pyomo.Dae — ***Robert Parker**, Bethany Nicholson, John Siirola, Lorenz Biegler*
4:45 Paper 40f: Pyddsbb: A Python Package for Simulation-Optimization Using Data-Driven Branch-and-Bound Techniques — *Jianyuan Zhai, **Suryateja Ravutla**, **Fani Boukouvala***
5:00 Paper 40g: Totally Open Pressure Swing Adsorption Intensification Laboratory (toPSAil) — ***Taehun Kim**, Joseph K. Scott*
5:15 Paper 40h: EAGO.jl: Next Generation Global & Robust Optimization in Julia, Revisited — ***Matthew Wilhelm**, Robert Gottlieb, Matthew Stuber*

(41) Systems Biology Approaches to Cancer

Sunday, Nov 7, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 109

Steven Abel, Co-Chair
Belinda Garana, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

3:30: Break
3:48 Paper 41a: The Landscape of Metabolic Pathway Dependencies in Cancer Cell Lines — ***Belinda Garana**, James Joly, Brandon Chew, Nicholas Graham*
4:06 Paper 41b: Metabolic Modeling to Explore the Landscape of Pancreatic Ductal Adenocarcinoma Cells in Diverse Physiological Conditions— ***Mohammad Mazharul Islam**, Andrea Goertzen, Rajib Saha*
4:24 Paper 160y: Single Cell Microwell Immunoassay for Quantitative Immune Response Monitoring — ***Qingxuan Li**, Sidi A Bencherif, Ming Su*
4:42 Paper 41f: The Effect of Metastasis Merging on Tumor Spread in the EMT6 Mouse Model — ***Isaac Pulatov**, Adeyinka Lesi, Madeleine Benguigu, Yuval Shaked, David Rumschitzki*
5:00 Paper 160ba: Towards Integrative Mechanistic Models of Mammalian Cell Responses to Anti-Cancer Drug Combinations — ***Cemal Erdem**, Arnab Mutsuddy, William Dodd, Marc R. Birtwistle*
5:18 Paper 41g: Can Soft Signals Turn Oncogenic? a Soft-Matter and Multiscale Modeling Approach to Engineering Cancer Cells and Inform Therapies (Invited Speaker) — ***Ravi Radhakrishnan***

(42) Systems Developmental Biology and Differentiation

Sunday, Nov 7, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 107

Gregory Reeves, Co-Chair
Bomyi Lim, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

3:30 Paper 42a: A Microfluidics-Based *in Vitro* Model of Anterior-Posterior Gut Patterning — ***Kiara Cui**, Leeya Engel, Kevin Liu, Kyle Loh, Lay Teng Ang, Alexander R. Dunn*
3:48 Paper 42h: 3D Inter-Allelic Competition Can Decrease the Total mRNA Production in Wild Type Embryos — ***Bomyi Lim***
4:06 Paper 42c: Using Machine Learning to Map Gene Regulatory Networks— ***Prasad Bandodkar**, Lossie (Elle) Rooney, Samiul Haque, Cranos Williams, Gregory Reeves*
4:24 Paper 42d: From Spikes to Intercellular Waves: Tuning Intercellular Ca^{2+}Signaling Dynamics Modulates Organ Size Control — ***Dharsan Soundarrajan**, Francisco Huizar, Ramezan Paravitorghabeh, Trent Robinett, Jeremiah J. Zartman*
4:42 Paper 42e: Investigating the Role of DNA-Protein Binding in Regulating Developmental Gene Expression in *Drosophila* embryos — ***Sahla Syed**, Bomyi Lim*
5:00 Paper 42f: Interpreting Positional Information in the Developing Organ of Corti — ***Matthew Thompson**, Vidhya Munnamalai, David Umulis*
5:18 Paper 42g: Integrating Fluidics, Imaging and Modeling to Analyze and Control Developmental Systems (Invited Speaker) — ***Jeremiah J. Zartman***

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

Sunday, Nov 7, 3:30 PM
Sheraton Back Bay, Republic Ballroom B

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

Sponsored by: Professional Development Committee Liaison

(44) Workshop: Social Justice and Chemical Engineering

Sunday, Nov 7, 3:30 PM
Sheraton Back Bay, Liberty B/C

Donna Riley, Co-Chair
Sindia M. Rivera-Jimenez, Co-Chair
Daniel Lepek, Co-Chair

Sponsored by: Education

(45) 3D Printing in Catalysts, Reaction, and Energy Industry

Monday, Nov 8, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 202

Lin Li, Chair
Kuochen Tsai, Co-Chair

Sponsored by: 3D Printing

8:00 Paper 45a: On Demand Ceramic Open Cell For Intensified Reaction By High Precision Additive Manufacturing — *Sang-Hoon Nam, Gian Han, Kavin Kowsari, **Nicholas X. Fang**, Seok Kim, Young Tae Cho*
8:40 Paper 45b: Additive Manufacturing of Hierarchical Porous Structures for Controlled Gas Bubble Flows Using Cellular Fluidics — ***Jonathan Davis**, Anna Guell Izard, Hawi Gemeda, Erika Fong, Joshua R. DeOtte, Nikola Dudukovic, Sarah Baker, Eric B. Duoss*
9:05 Paper 45c: Cellular Fluidics: Tuning Multiphase Interfaces in 3D Using Architected Porous Media — ***Nikola Dudukovic**, Erika Fong, Hawi Gemeda, Jonathan Davis, Sarah Baker, Eric B. Duoss*
9:30 Paper 45d: CO_2 Capture Modeling with Intrastage Cooling — ***Joshua Thompson**, Gyoung Gug Jang, Costas Tsouris*
9:55 Paper 45e: Thermal Energy Regulation with 3D Printed Polymer-Phase Change Material Composites — ***Peiran Wei**, Ciera Cipriani, Emily Pentzer*

(46) Active Colloidal Systems

Monday, Nov 8, 8:00 AM
Sheraton Back Bay, Back Bay Ballroom A

Bhuvnesh Bharti, Chair
Ilona Kretzschmar, Co-Chair
Ubaldo M. Córdova-Figueroa, Co-Chair

Sponsored by: Interfacial Phenomena

8:00 Paper 46a: Mechanisms of Transport Enhancement for Self-Propelled Nanoswimmers in a Porous Matrix — ***Haichao Wu**, Ben Greydanus, Daniel K. Schwartz*
8:20 Paper 46b: A Mechanical Theory of Nonequilibrium Phase Coexistence and Its Application to Motility-Induced Phase Separation — ***Hyeongjoo Row**, Ahmad Omar, Stewart Mallory, John Brady*
8:40 Paper 46c: Patchy Microellipsoids: Fabrication and Electric Field-Driven Active Propulsion — ***Jin Gyun Lee**, Ahmed Al Harraq, Kyle Bishop, Bhuvnesh Bharti*
9:00 Paper 46e: Multimodal Microwheel Swarms Targeting in Three-Dimensional Networks — ***Coy Zimmermann**, Keith B. Neeves, David W. M. Marr*
9:20 Paper 46f: Synchronization Behaviors of Active Oscillating Particles— ***Allan Brooks**, Jing Fan Yang, Albert Tianxiang Liu, Michael S. Strano*
9:40 Paper 46g: Play. Pause. Rewind. Measuring Local Entropy Production and Extractable Work in Active Matter. — *Buming Guo, Sunghan Ro, Aaron Shih, Average Phan, Robert Austin, **Stefano Martiniani**, Dov Levine, Paul M. Chaikin*

(47) Advanced batteries I

Monday, Nov 8, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 306

John Ekerdt, Chair
Jane Chang, Co-Chair

Sponsored by: Material Interfaces as Energy Solutions

8:00 Paper 47a: Delineating and Controlling the Electrode-Electrolyte Interfacial Reactions in High Energy Density Batteries — ***Arumugam Manthiram***
8:50 Paper 47b: Investigating Li-Ion Behavior in ALD Coated NMC Cathode Materials Via Molecular Dynamics — ***Julie Nguyen****, Krishan Kanhaiya, Katarina Odak, Hendrik Heinz, Alan Weimer*
9:15: Break
9:40 Paper 358d: Reserve Lithium-Ion Batteries for Lithium-Ion Free Cathodes— ***Mihit Parekh****, Manikandan Palanisamy, Vilas G. Pol*

(48) Advanced Treatment Technologies for Water

Monday, Nov 8, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 308

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

Sponsored by: Water

8:00 Paper 48a: Cobalt (II) Activated Sodium Percarbonate for the Degradation of Tetracycline Antibiotics By Using Reactive Oxygen and High Valent-Cobalt Oxo Species. — ***Muhammad Danish****, Usman Farooq, Sajjad Ahmad, Syed Waqas Ahmad, Shuguang Lu*
8:15 Paper 48b: Reactions of Viral Genomes during Disinfection and Advanced Oxidation: Kinetics and Product Identification. — ***Aleksandra Szczuka****, Krista Wigginton*
8:30 Paper 48c: Catalytic Capacitive Deionization for Adsorption and Reduction of Aqueous Nitrate — ***Tanya Rogers****, Sujin Guo, Leslie Arrazolo, Sergi Garcia-Segura, Michael S. Wong, Rafael Verduzco*
8:45 Paper 48d: Effective Municipal Wastewater Treatment at Low-Cost Using Coagulation/Precipitation Followed By Nano-Disinfection — ***Mohamed Mostafa****, Ahmed S. Mahmoud, Mohamed T. Kamar, Maha M. El-Shafei, M. Moussa,****Robert Peters***
9:00 Paper 48e: Degradation of Phenol Derivatives Using Advanced Oxidation Process in Batch and Continuous Film Reactors — ***Mayur Yenkie***
9:15 Paper 48f: Bioelectrochemical Sulfate Reduction Enhanced Nitrogen Removal from Industrial Wastewater Containing Ammonia and Sulfate — ***Jiaqi Ren****, Gaoming Wu, Zhongjian Li*
9:30 Paper 48g: Metal Single-Atom Catalysts Driven Heterogeneous Electro-Fenton Technology for Fast Elimination of Refractory Contaminants — ***Xie Quan****, Peike Cao*
9:45 Paper 48h: Ultra-Fine Heterogeneous Reduced Graphene Oxide Supported Zero Valent Iron-Copper Bimetallic Composite for the Efficient Degradation of Antibiotic Sulfamethoxazole — ***Muhammad Danish****, Usman Farooq, Sajjad Ahmad, Syed Waqas Ahmad, Shuguang Lu*

(49) Advances in Life Cycle Assessment

Monday, Nov 8, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 311

Vikas Khanna, Chair
Bhavik Bakshi, Co-Chair
Tapajyoti Ghosh, Co-Chair

Sponsored by: Sustainability Science and Engineering

8:00 Paper 49a: Toward Rapid Chemical Process-Based Life Cycle Inventory Data Generation: From Modeling Frameworks to Simulation to Machine Learning — ***Abhijeet Parvatker****, ****Matthew Eckelman***
8:20 Paper 49b: Planetary Boundaries, Ecosystem Services, and Life Cycle Assessment – Novel Insight By a Case Study and Computational Framework— ***Ying Xue****, Bhavik Bakshi*
8:40 Paper 49c: Estimating the Greenhouse Gas Emissions Payback Period of Planned Offshore Wind Energy Using Multiregional, Environmentally Extended Input-Output Analysis — ***Isha Sura****, Miriam Stevens, Shweta Singh, Apoorva Bademi*
9:00: Break
9:20 Paper 49e: Design and Environmental Assessment of an Ionic-Liquid-Based R407F Refrigerant Separation Process — *Daniel Jovell, Josep Oriol Pou Ibar,* ***Felix Llovell****, Rafael González-Olmos*
9:40 Paper 49f: A Hierarchical Techno-Ecological Decision Procedure for Sustainable Design — ***Michael Charles****, Bhavik Bakshi*

(50) Advances in Lignin Degradation Strategies

Monday, Nov 8, 8:00 AM
Marriott Copley Place, Exeter

Sunkyu Park, Chair

Sponsored by: Forest and Plant Bioproducts Division

8:00 Paper 50a: Towards a New Understanding of the Retro-Aldol Reaction for Oxidative Conversion of Lignin to Aromatic Aldehydes and Acids — ***Ajinkya More****, Thomas Elder, Zhihua Jiang*
8:15 Paper 50b: Lignin Depolymerization in a Molten Salt Hydrate (lithium bromide trihydrate) — ***Xuejun Pan***
8:30: Break
8:45 Paper 50d: Direct Catalytic Conversion of Lignocellulosic Biomass into Liquid Paraffins and Aromatics — *Prashant Niphadkar,* ***Ana Colaco Morais****, Vijay Bokade, Leonardo D. Sousa*

(51) Applications of Data Science in Molecular Sciences I

Monday, Nov 8, 8:00 AM
Marriott Copley Place, Salon H/I

Andrew Ferguson, Chair
Johannes Hachmann, Co-Chair
Andrew White, Co-Chair

Sponsored by: Applications of Data Science to Molecules and Materials

8:00 Paper 51a: Deep Learning Quantum Reaction Rate Constants— ***Stephanie Valleau***
8:25 Paper 51l: Building Blocks for Autonomous Computing Materials: Dimers, Trimers and Tetramers — ***Xingfei Wei***
8:37 Paper 51c: A Novel Machine Learning Model for the Accurate Design of Highly Selective Zeolitic-Imidazolate Frameworks — ***Ioannis Economou****, Panagiotis Krokidas, Stelios Karozis, George Giannakopoulos, Michael Kainourgiakis, Theodore Steriotis*
8:49 Paper 51d: Designing and Synthesizing Novel Dye Molecules Using Generative Modeling and Data-Driven Synthesis Planning — ***Camille Bilodeau****, Brent Koscher, Kevin P. Greenman, Rafael Gómez-Bombarelli, Klavs F. Jensen*
9:01: Break
9:13: Break
9:25 Paper 51g: Predicting Critical Micelle Concentrations for Surfactants Using Graph Convolutional Neural Networks — ***Shiyi Qin****, Tianyi Jin, Reid Van Lehn, Victor M. Zavala*
9:37: Break
9:49 Paper 51i: Cript: Establishing and Harnessing a Polymer Database— ***Dylan Walsh****, Tzyy-Shyang Lin, Chris Borg, Eric Muckley, Vinay Hegde, Ken Kroenlein, Klavs F. Jensen, Bradley Olsen*
10:01: Break
10:13 Paper 51k: Predicting Adhesive Free Energies of Polymer-Surface Interactions with Machine Learning — ***Jiale Shi****, Michael Quevillon, Jonathan K. Whitmer*

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

Monday, Nov 8, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 309

Marwa El-Sayed, Chair
Kerry Kelly, Co-Chair

Sponsored by: Air

8:00 Paper 52a: Modeling the Source Sectors Contribution to Nitrogen Deposition in U.S. Hydrological Regions — ***Kristina Wagstrom****, Sharmin Akter*
8:15: Break
8:30 Paper 52c: High Performance Air Assisted Flare Design to Handle Purge Flow Conditions — ***Hayder Alhameedi****, ASO Hassan, Qasim Al-Naddaf, Joseph D. Smith*
8:45 Paper 52d: Evaluating the Accuracy of UAV-Based Measurements through Experiments and Computational Fluid Dynamics Simulations. — ***Hayden Hedworth****, John Sohl, Tony Saad*
9:00 Paper 52e: On the Impact of COVID-19 Lockdowns on Air Quality and Transportation Patterns in Florida — ***Marwa El-Sayed***
9:15 Paper 52f: Understanding the Impacts of COVID-19 on Particle Pollution Using a Low-Cost Sensor Network — ***Kerry Kelly****, Ember Chadwick, Katrina Le, Anthony Butterfield, Tofigh Sayahi, Zheyuan Pei*
9:30 Paper 52g: The Influence of Atmospheric 'Blocking Signature' on Urban Particulate Matter ($PM_{2.5}$ and PM_{10}) and Trace Gases Characteristics of the City: Nur-Sultan, Central Kazakhstan — ***Gulden Ormanova****, Ferhat Karaca, Mehdi Amouei Torkmahalleh*

(54) Biomaterials: Faculty Candidates II

Monday, Nov 8, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 103

Whitney Stoppel, Chair
Bret Ulery, Co-Chair
Ryan Koppes, Co-Chair
Iman Noshadi, Co-Chair

Sponsored by: Biomaterials

8:00 Paper 54a: Design and Development of Intravenously Administered Hemostats to Target Hidden Wounds — ***Wontae Joo****, Celestine Hong, Bradley Olsen*
8:18 Paper 54b: Asymmetric Microcapsules for Osmotic Pressure Triggered Release of Biomolecules — ***Weixia Zhang****, David A. Weitz*
8:36: Break
8:54 Paper 54d: Temporally Controlled Release of Periosteal Paracrine Factor Mimetics for Efficient Bone Allograft Healing: A Cell and Growth Factor Free Approach — ***Sayantani Basu****, Amy Van Hove, Yiming Li, Danielle Benoit*
9:12 Paper 54e: Hierarchical Structure and Organization of Synthetic and Biopolymer Systems for the Advancement of Functional Material Development— ***Gabriel Burks***
9:30 Paper 54f: Programming Biomaterial Self-Assembly to Advance Molecular Robotics and Gene Delivery — ***Alexander Marras****, Carlos E. Castro, Matthew V. Tirrell*
9:48 Paper 54g: Bio-Inspired Soft Responsive Coatings for Natural and Synthetic Fibers — ***Bavand Keshavarz****, Gareth H. McKinley, Niels Holten-Andersen*
10:06 Paper 54h: Synthetic Brochosomes As Ultra-Antireflective, Super-Hydrophobic Biomimetic Materials in Multifunctional Films — ***Progna Banerjee****, Gabriel Burks, Marianne Alleyne, Mostafa Nassr, Sarah Bialik, Elizabeth Bello, Benny D. Freeman, Jeffrey E. Barrick, Charles M. Schroeder, Delia Milliron*

(55) Biomaterials for Drug Delivery: Cancer Therapies

Monday, Nov 8, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 209

Michael Gower, Chair
Rong Yang, Co-Chair
Lisa Volpatti, Co-Chair
Ashish Kulkarni, Co-Chair

Sponsored by: Biomaterials

8:00: Delayed Start
8:36 Paper 55a: Substrate Stiffness Regulates CD44 Receptor Mediated Endocytosis of Liposomal Nanoparticles — *Stephen L. Hayward, **Rashi Porwal**, Vaishaali Natarajan, David M Francis, Srivatsan Kidambi*
8:54 Paper 55b: ICAM-1 Nanobody Density on Liposomes Affects Selectivity for Triple Negative Breast Cancer and Inflamed Endothelium — ***Jacob Hebert**, Debra Auguste*
9:12 Paper 55c: Stimuli-Responsive Polycationic Nanogels for miRNA Delivery in the Treatment of Glioblastoma Multiforme — ***Deidra M. Ward**, Nicholas Peppas*
9:30 Paper 55f: Targeted Delivery of Self-Assembling ssDNA-Amphiphile Nanotubes to Glioblastoma — ***Zachary Schneiderman**, Efrosini Kokkoli, Huihui Kuang, Kevin Liaw, Clark Chen, Beibei Xu, Rangaramanujam Kannan*
9:48 Paper 55g: Implantable Optical Fibers for Delivering Immunotherapies and Tumor Impedance Measurement — ***Rong Tong***

(56) Biomolecular Engineering and Analyses to Understand Cell Migration, Membrane Components, and Genomic Structure

Monday, Nov 8, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 108

Kate Galloway, Co-Chair
Xiaoping Bao, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

8:00 Paper 56a: A New Strategy for Rapid Identification of DNA Zip Codes Via Targeted Rewiring of Endogenous Loci in Mammalian Cells — ***Meng Zhang**, Andrew Belmont, Huimin Zhao*
8:18 Paper 56b: Identification of Heterochromatin Markers As Epigenetic Drivers of Neuroendocrine Prostate Cancer (NEPC) Using Single Cell Tracking and Supervised Learning — ***Han Zhao**, Junkai Xie, Chongli Yuan*
8:36 Paper 56c: Polarized Ion Channels Regulate Migration Direction and Efficiency in Confinement — ***Yuqi Zhang**, Runchen Zhao, Panagiotis Mistriotis, Kaustav Bera, Konstantinos Konstantopoulos*
8:54 Paper 56d: Structured and Intrinsically Disordered Domains within Amphiphysin1 Work Together to Sense and Drive Membrane Curvature— ***Wade Zeno**, Jeanne C. Stachowiak*
9:12 Paper 56e: Tunable Enzymatic Synthesis of the Immunomodulator Lipid IV$_a$ to Enable Structure-Activity Analysis — ***Karthik Sankaranarayanan**, Xirui X. Antaris*, Brad A. Palanski, Abrahim El Gamal, Camilla M. Kao, William L. Fitch, Curt R. Fischer, Chaitan Khosla*
9:30 Paper 56h: Engineering Modular, Portable RNA-Based Control Systems for Cellular Reprogramming — ***Kate Galloway***
9:48 Paper 56g: Proprioception in Bacteria (Invited Speaker) — ***Pushkar Lele***

(57) Chemical Recycling of Waste Plastics I

Monday, Nov 8, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 205

Hilal Ezgi Toraman, Chair
Wan-Ting Chen, Co-Chair
Sheima Khatib, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

8:00 Paper 57a: Mechanistic Models of Polymer Degradation Chemistry— ***Linda Broadbelt***
8:30 Paper 57b: Tracking the Elementary Kinetics and Molecular Structures during Polyolefin Pyrolysis — ***Ziwei Wang**, Matthew Neurock, Isaac Mastalski, Nathan Sidhu, Paul Dauenhauer*
8:50 Paper 57d: Micropyrolysis of Polyethylene and Polypropylene: The Effect of Reactor Temperature and Vapor Residence Time on Product Distribution Prior to Bioconversion — ***Daniel Kulas**, Ali Zolghadr, Emily Byrne, Stephen Techtmann, David Shonnard*
9:10 Paper 57e: Lumped Product Kinetic Model of Plastics – Biomass Mixtures during Hydrothermal Liquefaction — ***Seshasayee Mahadevan Subramanya**, Abbey J. Kollar, Joyce Meiyi Yin, Rachel Stofanak, Lucas Powers, Katherine Maloney, Phillip E. Savage*
9:30 Paper 57f: Hydrothermal Process of the Ocean-Bound Plastic Waste into Value-Added Aromatic Chemicals — ***Taofeng Lu**, Wan-Ting Chen*
9:50 Paper 57g: Controlled Depolymerization and Upcycling of PVC — *Jason Bara, **ALI Alshaikh**, David McEachern, James W. Bridges, Kathryn E. O'Harra, Paul A. Rupar*
10:10: Break

(58) Continuous Drug Substance and Drug Product – Single Unit Operations - Session 1

Monday, Nov 15, 8:00 AM
Virtual, Pharmaceutical Discovery, Development and Manufacturing Forum (26)

Elcin Icten Gencer, Chair
Pallavi Pawar, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

8:00 Paper 58a: Developing a Workflow for Continuous Centrifugal Extraction— ***Eric Moschetta**, Benjamin Rizkin*
8:20 Paper 117d: A Scalable Continuous Reaction and Isolation Process for the Production of Sulfonyl Chloride Pharmaceutical Intermediates — ***Matthew Glace**, Cameron Armstrong, **Michael Scott**, Thomas Roper*
8:40 Paper 58c: Target Polymorphic Form Development Via Continuous Combined Cooling and Antisolvent Crystallization Using Oscillatory Baffled Crystallizer — ***Shivani Kshirsagar**, Naga Lakshmi Ramana Susarla, Srividya Ramakrishnan, Zoltan Nagy*
9:00 Paper 58d: Development of a Novel Continuous Spatially Distributed Diafiltration Unit Operation — ***Xiaoyan Long**, Zoheb Khan, Eoin Casey, Denis Dowling, **Steven Ferguson***
9:20 Paper 185a: Predicting Screw Feeder Flow Rates from Powder Properties and Operating Conditions — ***Brad Johnson**, Bram Bekaert, Valérie Vanhoorne, Thomas De Beer, Salvador Garcia-Munoz, Nikolaos Sahinidis*
9:40 Paper 185b: Model-Based Analysis of Breakage in Fluid Bed Drying of Continuously Produced Pharmaceutical Wet Granules — ***Michael Ghijs**, Tuur Vandeputte, Marie Vandromme, Selien Van Langenhove, Thomas De Beer, Ingmar Nopens*
10:00 Paper 185f: Development of a DEM-Based Digital Twin of a Continuous Direct Compression Line — *Peter Toson, **Pankaj Doshi**, Peter Bohling, Martina Trogrlic, MSc, Marko Matic, Daniel O. Blackwood, Kai Lee, Marta Moreno Benito, James Kimber, Hugh Verrier, Johannes G. Khinast, Dalibor Jajcevic*

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

Monday, Nov 8, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 313

Dharik Mallapragada, Chair
Christos Maravelias, Co-Chair
Arpa Ghosh, Co-Chair

Sponsored by: Sustainable Energy

8:00: Break
8:15 Paper 59b: Energia - an Integrated Framework and Software Prototype for Multiscale Energy Systems Transition Modeling, Optimization and Scenario Analysis — ***Rahul Kakodkar**, Cory Allen, Stefanos Baratsas, Marcello Di Martino, Styliani Avraamidou, C. Doga Demirhan, Clara F. Heuberger, Mark Klokkenburg, Efstratios N. Pistikopoulos*
8:30: Break
8:45 Paper 59d: Distributed and Sustainable Hydrogen Economy Via Renewable-Integrated and Intensified Process Design and Optimization — *Akhil Arora, **Manali S. Zantye**, M M Faruque Hasan*
9:00 Paper 59e: Unlocking the Potential of Open-Ocean Wind Energy Via Green Offshore Ammonia Production — ***Hanchu Wang**, Prodromos Daoutidis, Qi Zhang*

(61) Diagnostic Technologies for Clinical Applications

Monday, Nov 8, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 111

Piyush Jain, Chair
Chang Liu, Co-Chair

Sponsored by: Bioengineering

8:00 Paper 61a: A Rapid, Accurate, Scalable and Portable Testing (SPOT) System for COVID-19 Diagnosis — ***Guanhua Xun**, Stephan Thomas Lane, Vassily Andrew Petrov, Brandon Elliott Pepa, Huimin Zhao*
8:17 Paper 61b: An Ultrasensitive Flow-Based Digital ELISA for Detection of Attomolar Protein Concentrations — ***Connie Wu**, Tyler Dougan, David Walt*
8:34 Paper 61c: Novel Electrochemical Biosensor Using Small Binding Proteins for Early Detection of Aggressive Disease — ***Sunanda Dey**, David Hickey, Daniel Woldring*
8:51 Paper 61d: Deep Learning for Precise Breast Cancer Diagnosis and Risk Stratification: A Multi-Institutional Study — ***Shachi Mittal**, Rohit Bhargava*
9:08 Paper 61e: Detecting Intact Virus with Oligonucleotide Labels — *Thomas R. Carey, **Molly Kozminsky**, Jennifer Hall, Valerie Vargas-Zapata, Kristina Geiger, Laurent Coscoy, Lydia L. Sohn*
9:25 Paper 61f: Detection of Low-Level Tuberculosis Biomarkers in Patient Breath Utilizing Extracted Ion Chromatograms in GCMS Analysis — ***Mary Jeppson**, Christina Willis, Lani McKinnon, Tyler Gee, Emily Mei, Swomitra Mohanty*
9:42 Paper 61g: Proteomics-Informed Identification of Luminal Targets for in Situ Diagnosis of Inflammatory Bowel Disease — ***Shno Asad**, Christine Wegler, David Ahl, Christel A.S. Bergström, Mia Phillipson, Per Artursson, Alexandra Teleki*
9:59 Paper 61h: Nanoplasmonic Quantification of Pathogen-Derived Extracellular Vesicles in Plasma Microsamples — ***Tony Hu***

(62) Division Plenary: CAST (Invited Talks)

Monday, Nov 8, 8:00 AM
Sheraton Back Bay, Back Bay Ballroom C

Mario Eden, Chair
Alexander Mitsos, Co-Chair

Sponsored by: Computing Systems and Technology Division

8:00 Paper 62a: CAST Update — ***Mario Eden***
8:10 Paper 62b: CAST Programming Update — ***Alexander Mitsos***
8:20 Paper 62c: From Data to Process Design: Modeling Azeotropic Separation of High Global Warming Potential Hydrofluorocarbon Refrigerants Using Ionic Liquids — *Alejandro Garciadiego, Bridgette Befort, Gabriela Franco, **Alexander Dowling**, **Edward J. Maginn***
8:45 Paper 62d: Three Emerging Technologies That Will Soon Disrupt Manufacturing and Process Control — ***Thomas Badgwell**, R Donald Bartusiak*
9:10 Paper 62e: Discrete-Continuous Scheduling Algorithm: A Branch and Cut Approach — *Shamik Misra, **Christos Maravelias***
9:35 Paper 62f: A Stochastic Approximation Method for Approximating the Efficient Frontier of Chance-Constrained Nonlinear Programs — ***Rohit Kannan**, James Luedtke*

10:00 Paper 62g: Hybrid Gaussian Process Regression for Improved Predictability, Interpretability and Extrapolation — *Jinhyeun Kim, Christopher O. Luettgen, Kamran Paynabar,* ***Fani Boukouvala***

(63) Division Plenary: Gerhold and Kunesh Awards on Separations (Invited Talks)

Monday, Nov 8, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 304

Ranil Wickramasinghe, Chair
Anand Vennavelli, Co-Chair

Sponsored by: Separations Division

8:00 Paper 63a: Hollow Fiber or Spiral Wound Modules? — ***Glenn Lipscomb***
8:30 Paper 63b: Evolution of Distillation Equipment Technology and Future Development — ***Tony Cai***
9:00 Paper 63c: Chemistry & Engineering of Two-Dimensional Materials for Energy-Efficient Molecular Separation — ***Kumar Varoon Agrawal***
9:30 Paper 63d: High-Temperature Carbon-Dioxide Perm-Selective Membranes— ***Jerry Y.S. Lin***
10:00 Paper 63e: Membrane Based Separations in Petrochemical Industry: Looking Back, Looking Forward — ***Dhaval Bhandari***

(64) Dynamic Processes at Interfaces

Monday, Nov 8, 8:00 AM
Sheraton Back Bay, Back Bay Ballroom D

Prajnaparamita Dhar, Chair
Vivek Sharma, Co-Chair

Sponsored by: Interfacial Phenomena

8:00 Paper 64a: Synergistic Enhancement of Marangoni Flows Driven By Surface Gradients of Binary Catanionic Surfactant Mixtures — ***Tsung-Lin Hsieh****, Stephen Garoff, Robert D. Tilton*
8:15 Paper 64b: Three-Dimensional Technique for Measuring Sag in Drying Coatings — ***Marola Issa****, Hairou Yu, Maria Chiara Roffin, James Gilchrist, Steven V. Barancyk, Reza Rock, Christopher L. Wirth*
8:30 Paper 64c: Understanding the Effect of Dilatational Rheology on Lung Surfactant and Their Inhibitors — ***Sourav Barman****, Steven Iasella, Joseph Zasadzinski*
8:45 Paper 64d: Dynamic Properties of Polyelectrolyte-Surfactant Complexes Regulate the Escape of Microdroplets Elastically Trapped in Thermotropic Liquid Crystals — *Michael Tsuei, Nicholas L. Abbott,* ***Xin Wang***
9:00 Paper 64e: Synergistic Effects of Nanoparticles and Surfactants on the Stability of Oil-Water Interface Under Compression — ***Tuan Vu****, Xuan Duy Thao Nguyen, Sepideh Razavi, Dimitrios Papavassiliou*
9:15 Paper 64f: Impact of like-Charge Surfactants on Compressional Mechanical Properties of Particle-Laden Interfaces — ***Elton Lima Correia****, Dimitrios Papavassiliou, Sepideh Razavi*
9:30 Paper 64g: Dynamics and Rheology of Polymer-Surfactant Association Complexes — ***Chenxian Xu****, Thomas Mazur, Vivek Sharma*
9:45 Paper 64h: Polymer-Surfactant Complex and Shear Mediated Non-Equilibrium Colloidal Deposition Trajectories — *Lechuan Zhang, Huda Jerri,****Michael A Bevan***

(65) Efficient Processing of Lignin to Bioproducts and Biofuels

Monday, Nov 8, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 303

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

Sponsored by: Green Process and Product Engineering

8:00 Paper 65a: Elucidating Metabolic and Regulatory Mechanisms of Microbial Aromatic Utilization for Lignin Valorization — *Jinjin Diao,* ***Tae Seok Moon***
8:30 Paper 65b: Depolymerization of Corn Stover Lignin with Bulk Molybdenum Carbide Catalysts — *Xiaojun Yang, Maoqi Feng, Jae-Soon Choi, Harry M. Meyer III,* ***Bin Yang***
9:00 Paper 65c: Developing a Multi-Target Alkali Sterilization Strategy to Facilitate Lignin Dispersion and Promote Biological Lignin Valorization — ***Zhi-Min Zhao****, Shuyang Zhang, Xianzhi Meng, Yunqiao Pu, Arthur J. Ragauskas*
9:30 Paper 65d: Demethylated Lignin As the Interface Enhancer in FDM 3D Printing for PA12 Composites — ***Shuyang Zhang****, Xianzhi Meng, Arthur J. Ragauskas*
10:00 Paper 65e: Biorenewable Chemical Production from Pyrolysate By Lactic Acid Bacteria — *Samuel Rothstein, Swastik Sen,* ***Thomas J. Mansell***

(66) Electrocatalysis and Photoelectrocatalysis II: Oxygen and Organic Electrocatalysis

Monday, Nov 8, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 203

Fanglin Che, Chair
Robert Warburton, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

8:00 Paper 66a: Atomistic Deficiency of Lattice Oxygen for High Catalytic Activity in the Oxygen Evolution Reaction — ***Cheng Zhang****, Fangfang Wang, Hong Yang*
8:18 Paper 66b: Challenges and Frontiers in Water Oxidation Catalyst Development — ***Astrid M. Mueller***
8:36 Paper 66c: Influence of pH on Oxygen-Evolution-Reaction Mechanism— ***Julie Fornaciari****, Lien-Chun Weng, Tuan Anh Pham, Cheng Zhan, Shaun Alia, Alexis Bell, Tadashi Ogitsu, Nemanja Danilovic, Adam Weber*
8:54 Paper 66d: Electrochemistry with Oxygen: Activity, Stability, and New Design Principles for the Next Generation of Electrocatalysis — ***Michal Bajdich***
9:12 Paper 66e: Towards an Atomistic Understanding of the Dissolution of Rutile Oxides in Electrocatalytic Water-Splitting — ***Abhinav Sankara Raman****, Aleksandra Vojvodic*
9:30 Paper 66f: Oxides Supported Transition Metal Single-Atom Catalysts for Oxygen Electrocatalysis — ***G. T. Kasun Kalhara Gunasooriya****, Jens K. Nørskov*
9:48 Paper 66g: Improving the Efficiency of Electrocatalytic Ozone Production with Catalyst Microstructure and Dopants — ***N. Harsha Attanayake****, Maureen Tang*
10:06 Paper 66h: Mechanistic Studies on the Electrocatalytic Reduction of Nitroaromatic Compounds — ***Andrew Wong****, Michael Janik*

(67) Electrochemical CO2 Conversion I

Monday, Nov 8, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 206

Mohammad Asadi, Chair
Manish Shetty, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

8:00 Paper 67a: Design Criteria for Solvent and Additive Choices to Facilitate Selective and Sustainable Electrocarboxylation. — ***Nathan Corbin****, Karthish Manthiram*
8:18 Paper 67b: Effect of Pressure and Temperature on Carbon Dioxide Reduction at a Plasmonically Active Silver Cathode — ***Elizabeth R. Corson****, Erin B. Creel, Robert Kostecki, Jeffrey J. Urban, Bryan McCloskey*
8:36 Paper 67c: Exploring How Collective Ionic Assembly Influences Electrochemical Carbon Dioxide Upgrading — ***Matthew Gebbie****, Beichen Liu*
8:54 Paper 67d: CO_x Electrochemical Reduction with Additive Molecules Towards Longer Chain Products — ***Kavitha Chintam****, Linsey Seitz*
9:12 Paper 67e: Synthesis of 'Microphone' Structured Bi-Cu Chalcogenide for Efficient Electrocatalytic CO_2 Reduction — ***Xue Han***
9:30 Paper 67f: DNA-Immobilized Electrocatalysts for Improved CO_2 Reduction Efficiency — ***Gang Fan****, Ariel Furst*
9:48 Paper 67g: Understanding the Effects of Catalyst Surface Area on Electrochemical CO_2 Reduction in Aqueous and Vapor-Fed Systems — ***Daniel Corral****, Dong Un (Daniel) Lee, Victoria Ehlinger, Stephanie Nitopi, Lei Wang, Jaime Aviles Acosta, Jeremy T. Feaster, Yi-Rung Lin, Sarah Baker, Eric B. Duoss, Victor Beck, Christopher Hahn, Thomas Jaramillo*

(68) Electrochemistry for Applications in Sustainability

Monday, Nov 8, 8:00 AM
Sheraton Back Bay, Commonwealth

William Tarpeh, Chair
Sneha Akhade, Co-Chair

Sponsored by: Electrochemical Fundamentals

8:00 Paper 68a: *Probing Relationships between Bulk and Local Environments to Understand Impacts on the Electrocatalytic Oxygen Reduction Reaction*— ***Brianna Ruggiero****, Linsey Seitz, Justin Notestein*
8:20 Paper 68b: Effect of Near-Electrode Additives on Electrokinetic Remediation of Brine Spills — ***Javen Weston***
8:40 Paper 68c: Remediating and Valorizing Nitrogen-Polluted Wastewaters Via Electrodialysis and Nitrate Reduction — ***William Tarpeh****,* ***Jinyu Guo****, Matthew J. Liu, Sarah Blair, Adam Nielander, Thomas Jaramillo*
9:00 Paper 68d: Stabilization of Source-Separated Urine Using Electrochemically Synthesized Hydrogen Peroxide — ***Philip Arve****, Sudeep C. Popat*
9:20: Break
9:30 Paper 68e: Kinetic Analysis of Electrochemical Lactonization of Ketones Using Water As the Oxygen Atom Source — ***Joseph Maalouf****, Kyoungsuk Jin, Dengtao Yang, Aditya Limaye, Karthish Manthiram*
9:50 Paper 68f: Feasibility of Demand Response for Electrohydrodimerization Reactions in the Chemical Industrie — ***Natasa Milojevic***
10:10 Paper 68g: Electrochemical Analysis of Redox Electrolytes Using Microelectrode Voltammetry Modeling — ***Alexis Fenton Jr.****, Bertrand J. Neyhouse, Kevin M. Tenny, Fikile R. Brushett*

(70) Environmentally Friendly Product and Process Development for Sustainability

Monday, Nov 8, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 300

Qiang Xu, Chair
Onkar Manjrekar, Co-Chair
Deboleena Chakraborty, Co-Chair

Sponsored by: Process Research and Innovation

8:00: Break
8:23: Break
8:46: Break
9:09 Paper 70d: A Sustainable and Scalable Technology to Produce High Performance Mesoporous Silicon for Lithium Ion Batteries — ***Maximilian Yan****, Jake Entwistle,* ***Siddharth Patwardhan***
9:32 Paper 70e: Innovative Conceptual Design for an Industrial Complex Coupling Allam Power Cycle, Air Separation Unit, Ammonia Production, and Fertilizer Manufacturing Processes — *Song Wang,* ***Ying Liu****, Qiang Xu*
9:55 Paper 70f: Parametric Study on Physicochemical Properties of Ozone Microbubble - Applications to Fresh Produce Washing — ***Haknyeong Hong****, Jiakai Lu*

(71) Environmental Sensors and Monitoring

Monday, Nov 8, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 200

Gang Fan, Chair
Kevin Cash, Co-Chair
Alice Gillen, Co-Chair
Katie Dongmei Li-Oakey, Co-Chair

Sponsored by: Sensors

8:00 Paper 71a: Invited Talk - Transmission Reduction Artificial Intelligence System (TRAIS) — ***Erica Forzani***, *Bhavesh Patel, Amelia Lowell, Kelly McKay, Gabriel Pyznar, Xiaojun Xian, Karam Abi Karam, Piyush Hota, Adithya Shyamala Pandam, Michael Serhan, Sabrina Jimena Mora*
8:25 Paper 71b: Invited Talk - Carbon Nanotubes As Near-Infrared Fluorescence Biosensors of Intracellular Trafficking and Wound Monitoring— ***Daniel Roxbury***, *Mohammad Moein Safaee, Mitchell Gravely*
8:50 Paper 71c: Mitigation of Positional-Dependent Limitations of Resonant Sensors and Applications Enabled Thereby — ***Yee Jher Chan***, *Adam Carr, Nigel Reuel*
9:07 Paper 71f: On-Board Timing, Memory, and Sensing in Autonomous Cell-Sized Robots Enabled By a Simple Memristor-Based Circuit — ***Jing Fan Yang***, *Albert Tianxiang Liu, Ge Zhang, Allan Brooks, Volodymyr Koman, Sungyun Yang, Pingwei Liu, Michael S. Strano*
9:24 Paper 71g: Detection of Benzene, Toluene, Ethylbenzene and Xylene in Air Using Micro-Preconcentrator/Solid Phase Micro-Extraction/Gas Chromatography Mass Spectrometry — ***Sujoy Halder***, *Zhenzhen Xie, Michael H. Nantz, Xiao-an Fu*
9:41 Paper 71h: Novel, Ultra-Small, Robust Electrochemical Sensor for in-Situ Detection of Cd(II) in the Environment — ***Muzammil Nishar Ahmed***, *Faieza Bodowara, Juliana Penteado, Laura Guidugli, Wendy Zhou, Pavithra Pathirathna*

(72) Fluidization: Fundamentals

Monday, Nov 8, 8:00 AM
Sheraton Back Bay, Fairfax A/B

Mayank Kashyap, Chair
Aaron Lattanzi, Co-Chair

Sponsored by: Fluidization and Fluid-Particle Systems

8:00 Paper 72a: Characterizing and Modeling Structured Bubbling in Gas-Solid Fluidized Beds — *Qiang Guo, Yuxuan Zhang, Azin Padash,* ***Christopher M. Boyce***
8:20 Paper 701a: Modeling of Taylor-Couette Vortices in Fluidized Beds— ***Christopher M. Boyce***
8:40 Paper 72b: Fluid-Mediated Sources to Granular Temperature in Homogeneous Fluidization — ***Aaron Lattanzi***, *Vahid Tavanashad, Shankar Subramaniam, Jesse Capecelatro*
9:00 Paper 72c: Effect of Particle Size on the Modulation of Near-Wall Turbulent Flow Structures in Particle-Resolved Direct Numerical Simulations and Eulerian-Lagrangian Simulations — ***Jonathan Van Doren***, *Mohamed H. Kasbaoui*
9:20 Paper 72f: Particulate Process and Product Design: Single Drop Granulation — ***Heather Emady***

(73) Fundamentals of Interfacial Phenomena II

Monday, Nov 8, 8:00 AM
Sheraton Back Bay, Back Bay Ballroom B

Dongjin Seo, Chair
Siamak Nejati, Co-Chair

Sponsored by: Interfacial Phenomena

8:00 Paper 73c: Magnetic Architecture of Colloidal Supraparticles — ***Ahmed Al Harraq***, *JinGyun Lee, Bhuvnesh Bharti*
8:15 Paper 73d: Wetting Transparency of Ultrathin Polymer Films — *Evon Petek,* ***Reika Katsumata***
8:30 Paper 73e: Liquid Crystal-Infused Porous Surfaces with Molecular Order-Dependent Slipperiness and Cargo Release — ***Xiaoguang WANG***, *Yang Xu, Adil Rather, Rajdeep Mamtani*
8:45 Paper 73g: Experimental Determination of the Hamaker Constants of Various Solid Materials with Improved Accuracy Using Atomic Force Microscopy— *Michael Stevenson, Stephen P. Beaudoin,* ***David Corti***
9:00: Break
9:15 Paper 73i: 3D Printable, Biodegradable Lignin-Zein Composite — ***Jin Gyun Lee***, *Ahmed Al Harraq, Bhuvnesh Bharti*
9:30 Paper 73j: Direct Observations of the Double-Layering Molecular Structure of Mica-Confined Ionic Liquids — ***Bingchen Wang***, *Lei Li*
9:45 Paper 640b: Effects of Cationic and Anionic Ions on Nanosurfactant Performance: Colloidal Stability and Interfacial Tension Study — ***Ahmed Wasel Alsmaeil***, ***Afnan Mashat***, *Mustafa Alsaffar, Amr Abdel-Fattah*

(74) Gas Hydrates Science and Engineering

Wednesday, Nov 17, 8:00 AM
Virtual, Thermodynamics and Transport Properties (01A)

Amadeu Sum, Chair
Praveen Linga, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

8:00 Paper 74a: Electrical Resistance Measurement during CH_4-CO_2 Mixed Hydrate Formation and Dissociation in Sandstone — ***Jyoti Shanker Pandey***, *Nicolas von Solms,* ***Qian Ouyang***
8:20 Paper 74b: Pore-Scale Study on the Effects of Hydrate Distribution Morphology on Dissociation Process Utilizing a Coupled Multiphase Hydrodynamic and Thermal Lattice-Boltzmann Model — ***Zhuoran Li***, *Guan Qin*
8:40 Paper 74c: Sustainable Methane Hydrate Formation Via Superabsorbent Polymers (SAPs) and Tetrahydrofuran (THF) — ***Dong Woo Kang***, *Wonhyeong Lee, Yun-Ho Ahn, Jae Lee*
9:00 Paper 74d: Molecular Dynamics Study for the Enhancement of Carbon Dioxide Exchange in Methane Hydrates. — ***Kavya Tadepalli***, *Rajnish Kumar*

(75) Industry 4.0, Digital Twins, and Digital Transformation II

Monday, Nov 8, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 201

Dhruv Gupta, Chair
Yuncheng Du, Co-Chair

Sponsored by: Next-Gen Manufacturing

8:00 Paper 75a: Keynote Talk - Industry 4.0: Continuous Pharmaceutical Manufacturing Process — ***Ravendra Singh***
8:30 Paper 75b: Adaptive Strategies for Updating Unit Operation Models and in-Line Monitoring of Blend Uniformity in Continuous Pharmaceutical Manufacturing Process — ***Yingjie Chen***, *Shashwat Gupta, Andres Roman-Ospino, Fernando Muzzio, Marianthi Ierapetritou*
8:50 Paper 75c: Data-Driven Approaches Towards Equipment Health-Classification and Predictive Monitoring in Drug Product Manufacturing— ***Philipp Zuercher***, *Sara Badr, Hirokazu Sugiyama*
9:10 Paper 75d: An Equation-Oriented Model of a Trickle-Bed Reactor for Hydrodesulfurization Process Analysis and Digital Twin Applications — ***Heleno Bispo***, ***Arianne Barros***, *Fernando V. Lima, Antônio Tavernard*
9:30 Paper 75e: Keynote Talk - S. J. Qin (Industry 4.0, Digital Twins, and Digital Transformation II) — ***S. Joe Qin***
10:00 Paper 75f: Keynote Talk - Dimitri Papageorgiou (Industry 4.0, Digital Twins, and Digital Transformation II) — ***Dimitri Papageorgiou***

(77) In Honor of the 2019 R.H. Wilhelm Award Winner I (Invited Talks)

Monday, Nov 8, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 210

C Franklin Goldsmith, Chair
Amrit Jalan, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

8:00 Paper 77a: Learning to Design Organic Syntheses — ***Connor Coley***
8:25 Paper 77b: Heavy Oil Hydroconversion: Modeling Composition and Chemistry — *Steven Pyl, Michael R. Harper, Richard J. Quann,* ***Sumathy Raman***
8:50 Paper 77c: Conversion of Methane to Value-Added Chemicals— ***Dionisios Vlachos***
9:15 Paper 134d: Rmg in 2D: Recent Advances in Automatic Mechanism Generation for Heterogeneous Catalysis — ***C Franklin Goldsmith***, *Richard H. West*
9:40 Paper 77e: Novel Reaction Pathways in Low-Temperature Oxidation: Applications in Liquid-Phase and Atmospheric Systems — ***Amrit Jalan***

(78) Leading Chemical Engineering in the Era of Increased Data Utilization (Invited Talks)

Monday, Nov 8, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 301

Cristina Thomas, Chair

Sponsored by: Management Division

8:00 Paper 78a: The Use of Digital Technologies in Materials and Process Design — ***Cristina Thomas***, *Jung-Sheng Wu*
8:30 Paper 78b: The Digital Transformation of the Chemicals Industry - and How to Prepare — ***Anthony Schiavo***
9:00 Paper 78d: Presentation 4 - Leading Chemical Engineering in the Era of Increased Data Utilization (Invited Talks) — ***Eric Lin***
9:30 Paper 78e: Presentation 5 - Leading Chemical Engineering in the Era of Increased Data Utilization (Invited Talks) — ***Cristina Thomas***

(79) Nanoscale Science and Engineering Forum Division Plenary

Monday, Nov 8, 8:00 AM
Marriott Copley Place, Wellesley

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

Sponsored by: Nanoscale Science and Engineering Forum

8:00: Introductory Remarks
8:30 Paper 79a: Electrifying CO2 into Fuels and Chemicals — ***Haotian Wang***
9:30 Paper 79b: Chemical Engineering of Chiral Nanostructures — ***Nicholas Kotov***

(80) Nanostructured Materials for Environmental Applications

Monday, Nov 8, 8:00 AM
Sheraton Back Bay, Hampton

Timothy M. Brenza, Chair

Sponsored by: Nanoparticles

8:00 Paper 80b: A Stimuli-Responsive, Hydrolysable Poly(Vinyl Laurate-co-Vinyl Acetate) Nanoparticle Platform for in Situ Release of Surfactants— ***Bashayer S. Aldakkan***, *Mohammed A. Hammami, Qi Genggeng, Mazen Kanj, Emmanuel P. Giannelis*
8:15 Paper 80c: Surface Characterization of Modified Fe_3O_4 Catalysts for Inductively Driven Alcohol Oxidation — ***Natalia da Silva Moura***, *Cameron Roman,*

Khashayar R. Bajgiran, Kerry M. Dooley, Adam Melvin, ***James Dorman***

(81) Particulate Systems: Solids and Processing: In-person

Monday, Nov 8, 8:00 AM
Sheraton Back Bay, Gardner

Aaron Morris, Co-Chair

Sponsored by: Solids Flow, Handling and Processing

8:00 Paper 81a: Heat Transfer in a Rotary Drum — ***Bhaumik Bheda****, Heather Emady*
8:15 Paper 81b: Scale-up of Heat Transfer for Rotary Drums with Baffles— ***Elaheh Ardalani****, William Borghard, Benjamin Glasser, Alberto Cuitiño*
8:30 Paper 81d: Continuum Modeling of Corn Stover Feedstock through a Compression Feed Screw — ***Abhishek Paul****, Marcial Gonzalez, Carl R. Wassgren*
8:45 Paper 81e: Starch Salt Composites; How to Reduce Water Uptake and Weakening — ***Gabrie M.H. Meesters****, Quinten Fung-A-Jou*
9:00 Paper 81f: Particle-Level Residence Times in a Twin-Screw Feeder— ***Peter Toson****, Johannes G. Khinast*

(82) Pioneers of Catalysis and Reaction Engineering (Invited Talks)

Monday, Nov 8, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 208

Bihter Padak, Chair
Sheima Khatib, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

8:00 Paper 82a: New High-Performance Hydrocracking Catalyst Platform— ***Sarika Goel***
8:30 Paper 82b: First-Principles Modeling of the Effect of Surface Modification Strategies on Hydrogenation Catalysis — ***Carrie Farberow***
9:00 Paper 82c: Building Catalysts, Reactors and Engineers for a Sustainable Future — ***Jeremy Feaster***
9:30 Paper 82d: Metal-Organic Frameworks (MOFs) As Catalysts and Catalyst Precursors for Oxidation and Reduction Reactions — ***Michele Sarazen***
10:00 Paper 82e: Probing Dynamic Materials and Systems for Electrocatalytic Processes — ***Linsey Seitz***

(83) Polymer Networks and Gels 2

Monday, Nov 8, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 104

Monirosadat Sadati, Chair
Jinhye Bae, Co-Chair
Nese Orbey, Co-Chair

Sponsored by: Polymers

8:00 Paper 83a: Random Liquid Crystalline Copolymers Consisting of Prolate and Oblate Liquid Crystal Monomers — ***Xiaoguang WANG****, Yang Xu, Robert Dupont*
8:15 Paper 83b: Hydrogel Swelling and Deswelling in Complex Environments— *Jean-Francois Louf, Galen Mandes, Nancy Lu, Tapomoy Bhattacharjee, Margaret G. O'Connell, H. Jeremy Cho,* ***Sujit Datta***
8:30 Paper 83d: Effect of Backbone and End-Group Regioisomerism on Thermomechanical Properties of Vanillin-Based Polyurethane Networks— ***Adithya Rangamani****, Christopher Alabi*
8:45 Paper 83e: Reactivity You Can Feel: Substituent Effects and Network Fracture — *Shu Wang,* ***Haley Beech****, Brandon H. Bowser, Tatiana B. Kouznetsova, Bradley Olsen, Michael Rubinstein, Stephen L. Craig*
9:00 Paper 83f: Versatile Platform for Synthesizing Polymer Membrane Libraries Using Functional Networks — ***Joshua Moon****, Rahul Sujanani, Zhishuai Geng, Benny D. Freeman, Rachel Segalman, Craig J. Hawker*
9:15 Paper 83g: Unentangled Vitrimer Melts: Generalized Rouse Theory Reveals Impact of Cross-Link and Backbone Chemistry on Linear Viscoelasticity— ***Ralm Ricarte****, Sachin Shanbhag*
9:30 Paper 83h: Designing a Resilin-like Retractable and Stretchable Hydrogel— *Rosa Maria Badani Prado, Satish Mishra, Buckston Morgan,* ***Santanu Kundu***
9:45 Paper 83i: The Dynamics and Mechanics of Inhomogeneous Polymer Networks — ***Robert Riggleman****, Han Zhang, Ziyu Ye*
10:00 Paper 83j: Sculpting Hydrogels Using Advective Assembly — ***Alexandra V. Bayles****, Tazio Pleij, Martin Hofmann, Jan Vermant*
10:15 Paper 83c: Dynamically Cross-Linked Polyolefin Elastomers with Highly Improved Mechanical and Thermal Performance — ***Yangke Xiao****, Pingwei Liu, Wen-Jun Wang, Bo-Geng Li*

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

Monday, Nov 8, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 101

Mary am Ende, Chair
John Thomas, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

8:00 Paper 84a: Predicting the Diameters of Droplets Produced in Turbulent Liquid-Liquid Dispersion — ***Francesco Ricci****, John Thomas, Brian DeVincentis, Johannes Wutz*
8:24: Break
8:48 Paper 84c: Computational Fluid Dynamics Study to Develop a Scale-up Strategy for Non-Newtonian Fluids in Pharmaceutical Industry — ***Nikhil Srivastava****, Saurav S. Rath, SVB Janardhan Garikipati, Birendra K. David*
9:12 Paper 84d: Modelling the Effect of Ice Nucleation Stochasticity on Batch Heterogeneity of Freezing Processes of Vials on a Shelf — ***Leif-Thore Deck****, Marco Mazzotti*
9:36 Paper 84f: API Crystallization Process Development for Improved Consistency, Bulk Properties, and to Enable Downstream Processing — ***Justin Quon****, Landon Durak, Charles D. Papageorgiou*
10:00 Paper 714d: Loss-in-Weight Control of a Low Dose Powder Feeding System — *Julia Kruisz,* ***Sarah Fathollahi****, Jakob Rehrl, Stephan Sacher, Johannes G. Khinast*

(85) Reactor Engineering for Biomass Feedstocks II

Monday, Nov 8, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 312

Yukihiko Matsumura, Chair
Kenichiro Tanoue, Co-Chair
Xianghong Qian, Co-Chair

Sponsored by: Sustainable Biorefineries

8:00 Paper 85a: Evaluation of Ultrasonic Pretreatment on Catalytic Hydrothermal Liquefaction of Woody Biomass — ***Max Lampert****, Bharath Maddipudi, Vinod Amar, Anuradha Shende,* ***Rajesh Shende***
8:15 Paper 85b: Development of a Novel Nickel-Ceramic Filter for Hot Gas Removal of Tars and Particulates from Biomass Syngas — ***Devin Peck***
8:30 Paper 85c: One-Pot Conversion of Biomass in Aprotic Solvent for Chemicals and Quality Lignin Based on Plasma Electrolysis — *Lusi A, Harish Radhakrishnan,* ***Xianglan Bai***
8:45 Paper 85d: Modeling Green Diesel Hydroprocessing Via Molecule-Based Reactor — ***Zhen Hou****, Lingxiang Li, Shu Wang, Lili Yu, Christopher Quan, Darin Campbell*
9:00 Paper 85e: Production of Short-Chain Oligomers from Cellulose Via Selective Hydrolysis in Molten Salt Hydrates and Separation — *Qiyu Liu,* ***Wei Fan***
9:15 Paper 85f: Conversion of Food Waste to Levulinic Acid Using a Catalytic Membranemembrane Reactor — ***Ranil Wickramasinghe****, Zhexi Zhu, Xianghong Qian*

(86) Spotlights in Thermodynamics and Computational Molecular Science (Invited Talks)

Monday, Nov 8, 8:00 AM
Marriott Copley Place, Salon J/K

M. Scott Shell, Chair
Arthi Jayaraman, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

8:00: Introductory Remarks
8:05 Paper 86a: Model for Disordered Proteins with Strongly Sequence-Dependent Liquid Phase Behavior — ***Antonia Statt****, Helena Casademunt, Athanassios Panagiotopoulos, Clifford P. Brangwynne*
8:28 Paper 86b: A Touch of Non-Linearity: Mesoscale Swimmers and Active Matter in Fluids — ***Daphne Klotsa****, Thomas Dombrowski, Hong Nguyen*
8:51 Paper 86c: Binary Solute Adsorption in Surfactant Bilayers with Gibbs Ensemble Monte Carlo Simulations — ***Mona Minkara***
9:14: Break
9:19 Paper 86d: Chemistry Under Extreme Conditions: Accelerating Research through Artificial Intelligence — ***Rebecca Lindsey***
9:42 Paper 86e: Modeling Diffusion Processes in the Zeolite Nanopores— ***Neeraj Rai****, Md Masrul Huda, Nusrat Jahan, Chinmoy Saha*
10:05 Paper 86f: Discovery of Novel Compounds and Pathways through Identification of Bioprivileged Molecules — ***Linda Broadbelt****, Lauren Lopez, Brent H. Shanks, Guanhua Wang, Matthew W. Coile, Yixuan Chen, John Torkelson*

(87) Free Forum on Engineering Education: First Year and Sophomore Year

Monday, Nov 8, 8:00 AM
Sheraton Back Bay, Liberty B/C

Daniel Burkey, Chair
Kristine Horvat, Co-Chair
Taryn Bayles, Co-Chair

Sponsored by: Undergraduate Education

8:00: Break
8:18: Break
8:36 Paper 87c: Evaluating Performance in a Summer Online Thermodynamics Course Using a Concept Inventory — ***David Silverstein****, Sarah Wilson*
8:54 Paper 87d: Engaging an Entrepreneurial Mindset Though Open-Ended Projects in the Sophomore Year — ***Kristine Horvat***
9:12 Paper 87e: Problem Solving When Textbook Problems Are Replaced with Student-Written Youtube Problems — ***Uchenna Asogwa****, T Ryan Duckett, Amanda P. Malefyt, Lindsey Stevens, Gale Mentzer, Matthew Liberatore*
9:30 Paper 87f: Addressing Student Equity in the First Year through the Student Experience Project — ***Glenn Lipscomb***

(88) Lessons Learned from Teaching Chemical Engineering Online I (How We Changed Our Courses)

Monday, Nov 8, 8:00 AM
Sheraton Back Bay, Republic Ballroom B

Christi Patton Luks, Chair
Fernando Merida, Co-Chair
Donald Visco Jr., Co-Chair

Sponsored by: Education

8:00 Paper 88a: Teaching Process Calculations to Undergraduate Chemical Engineers: An Engaged & Energized Online Class — ***Preeti Aghalayam****, Kartic Vaidyanathan*

8:18 Paper 88b: From MOOCs to Residential Instruction – Departmental Perspective on Digital Learning @ MIT ChE — ***Zongyu Gu***, *Martin Z. Bazant*
8:36 Paper 88c: Virtual Implementation of a Hands-on Learning Tool and Its Effect on Student Comprehension and Motivational Gains — ***Kitana Kaiphanliam***, *Olivia Reynolds, Aminul Islam Khan, Olufunso Oje, David B. Thiessen, Prashanta Dutta, Olusola Adesope, Jacqueline Burgher Gartner, Bernard Van Wie*
8:54 Paper 88e: Developing Simulation-Based, Student-Centred Educational Software in Process-Control Education and Training — ***Niall English***
9:12 Paper 88f: Reinventing Unit Operations Laboratories Post-COVID-19 — *Samira Azarin,* ***Christopher Barr****, Janie Brennan, Tracy Carter, Amy J. Karlsson, Sarah Wilson*

(89) Stem Cells and Tissue Engineering

Monday, Nov 8, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 110

Adrianne Rosales, Co-Chair
Quinton Smith, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

8:00 Paper 89a: Cell Engineering and Gene Editing Approaches Towards Correcting Human Skin Pigmentation Disorders — ***Vivek Bajpai, MD, PhD****, Tomek Swigut, Joanna Wysocka*
8:18 Paper 89b: *In Vitro* Tissue Model with Collagen and Aldehyde/Hydrazide-Modified Hyaluronic Acid Hydrogels — ***Jessica Torres****, Sathvik Madduri, Fanfei Meng, Kevin Buno, Yoon Yeo, Luis Solorio, Julie C. Liu*
8:36 Paper 89c: Wnt/BMP Regulates Multipotency of Neural Crest Stem Cells Via Metabolic and Epigenetic Rewiring — ***Pihu Mehrotra****, Izuagie Ikhapoh, Yali Zhang, Jianmin Wang, Pedro Lei, Song Liu, Stelios Andreadis*
8:54 Paper 89d: Enhancing Vascularized Biomimetic Organ and Tissue By Engineering Vascular Cells with Early Development Transcription Factor— ***DucHuy Nguyen****, Brisa Palikuqi, Sina Rabbany, Shahin Rafii, Robert Schwartz*
9:12 Paper 89h: Influencing Stem Cell Secreted Factors with Peptoid-Containing Biomaterials — ***Adrianne Rosales***
9:30 Paper 89f: Capturing Biomaterial Degradation and Tissue Formation Following Implantation of Silk-ECM Composite Sponges Using Machine Learning and Kinetic Modeling — *Julie F. Jameson, Joshua Peeples, Nisha Kotta, Jason Butler, Alina Zare,* ***Whitney Stoppel***
9:48 Paper 89g: A Simple Biomaterial for Diverse Tissue Engineering Applications (Invited Speaker) — ***Ethan Lippmann***

(90) Synthesis and Application of Inorganic Materials

Monday, Nov 8, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 105

Wei Fan, Chair
Rishabh Jain, Co-Chair
Aseem Chawla, Co-Chair
Kumar Varoon Agrawal, Co-Chair
Praveen K. Thallapally, Co-Chair

Sponsored by: Inorganic Materials

8:00 Paper 90a: Synthesis of Aluminoborosilicate Isomorphous to Zeolite Tun and Its Acidic and Catalytic Properties — *Feiyu Qin, Yong Wang, Yao Lu, Hermann Gies,* ***Toshiyuki Yokoi***
8:15 Paper 90b: Fabrication of Unique Aei-Type Aluminosilicate with Sheet-like Morphology — *Takashi Takeuchi, Ryota Osuga, Takeshi Matsumoto, Junko N. Kondo, Hermann Gies,* ***Toshiyuki Yokoi***
8:30 Paper 90c: Synthesis of Exsolvable Multi-Metallic Nanoparticles Using the Defect Chemistry of Perovskite Oxides — ***Kandis Leslie Abdul-Aziz****, Soham Shah, Mingjie Xu, Xiaoqing Pan*
8:45 Paper 90d: Multivalent Cations Function As Accelerants and Structure-Directing Agents of Zeolite Crystallization — ***Yu Liang****, Allan J. Jacobson, Jeffrey Rimer*
9:00 Paper 90e: Reactor Design Criteria for Reliable Kinetics in Zeolite Synthesis Via Micro-Scale Crystallization — ***Jacob Crislip***
9:15 Paper 90f: ZIF-8 Membrane Performance Modification *Via* Facile Vapor-Phase Metal-Organic Treatment — ***Dennis Lee****, Mikio Hayashi, Matheus Dorneles de Mello, Jorge Boscoboinik, Michael Tsapatsis*
9:30 Paper 90g: Performances of Coatings of Various Zeolites for Heating/Cooling Applications — ***Cigdem Atalay-Oral****, Melkon Tatlier*
9:45 Paper 90h: Synthesis and Transport Property of Hierarchical Siliceous Zeolites Synthesized By Post-Synthetic Surfactant Templating — ***Kaivalya Gawande****, Wei Fan, W. Curtis Conner Jr.*
10:00 Paper 90i: Solvent-Free Synthesis of Porous Organic Frameworks— ***Siamak Nejati***
10:15 Paper 90j: Correlating Ion Solvation and Conductivity in Porous Aromatic Frameworks — ***Kaitlyn Engler****, Jeffrey A. Reimer, Jeffrey R. Long*

(91) Systems Biology Methods and Technologies

Monday, Nov 8, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 107

Lily Cheung, Co-Chair
Siddharth Dey, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

8:00 Paper 91a: Graphical Model Framework for Automated Annotation of Cell Identities in Dense Cellular Images. — ***Shivesh Chaudhary****, Sol Ah Lee, Yueyi Li, Hang Lu*
8:18 Paper 91h: Mapping the Methylome in Single Cells Reveals Heterogeneity in DNA Methylation Turnover during Early Mammalian Development— ***Siddharth Dey***
8:36 Paper 91c: Quantitative Analysis of Transporter Activity Biosensors — *Jihyun Park,* ***Lily Cheung***
8:54 Paper 91d: FLOW-Cytometry Analysis Reveals Persister Resuscitation Characteristics — ***Sayed Golam Mohiuddin****, Pouria Kavousi, Mehmet Orman*
9:12 Paper 91e: Combined Physics and Bmp Signaling Network Dynamics to Model Early Embryonic Development in Zebrafish — ***Linlin Li****, Adrian Buganza Tepole, David Umulis*
9:30 Paper 91f: A CRISPR-Cas9 Screen for Systematic Discovery of Genes and Pathways Controlling Human Melanogenesis — ***Vivek Bajpai, MD, PhD****, Tomek Swigut, Joanna Wysocka*
9:48 Paper 91g: Towards Holistic Imaging and Rapid Phenotyping of Complex Biological Systems (Invited Speaker) — ***Kwanghun Chung***

(92) Topical Plenary: Fundamentals of Microbial Interactions with Interfaces (Invited Talks)

Monday, Nov 8, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 310

Elizabeth Stewart, Chair
Jessica Schiffman, Co-Chair

Sponsored by: Microbes at Biomedical Interfaces

8:00 Paper 92b: Vapor-Deposited Biointerfaces for Fouling Reduction and Regulated Microbial Behaviors — ***Rong Yang***
8:30 Paper 92c: Development of Biomimetic Nanostructured Surfaces to Combat Bacterial Adhesion and Growth without Antibiotic Treatments— ***Yeongseon Jang***
9:00 Paper 92d: Rapid Adhesion Testing of Biological Films By Laser-Induced Stress Wave Loading — ***Martha Grady***
9:30 Paper 92e: Spatiotemporal Analyte and Metabolic Tracking in Microbial Biofilms with Nanosensors — ***Kevin Cash***
10:00 Paper 92a: Bacterial Biofilms Sense and Response to Substrate Stiffness— ***Alison Patteson***

(93) Unconscious Bias

Monday, Nov 8, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 204

Eric Bell, Co-Chair
Sindia M. Rivera-Jimenez, Co-Chair

Sponsored by: Engineering for Inclusion

(96) Academia-Industry Partnership: What New Graduates Should Know

Monday, Nov 8, 11:00 AM
John B. Hynes Veterans Memorial Convention Center, 302

Richard Braatz, Chair
Lucas J. Landherr, Co-Chair

Sponsored by: Bridging the Skills Gap in Chemical Engineering

11:00 Paper 96a: Aligning What Industry and Academia Expect of New Graduates — ***Yang Luo****,* ***Phillip Westmoreland***
11:30: Discussion

(97) WIC Keynote Featuring Networking Breakfast and Poster Session - (Ticketed Event)

Monday, Nov 8, 9:00 AM
Sheraton Back Bay, Grand Ballroom

Lisa Volpatti, Chair

Sponsored by: Women in Chemical Engineering Committee (WIC)

(98) 2021 Hoover Medal Lecture

Monday, Nov 8, 12:15 PM
John B. Hynes Veterans Memorial Convention Center, Ballroom B

Maria Burka, Chair

Sponsored by: Awards Committee

12:15: Introductory Remarks
12:25 Paper 98a: "Black Lives Matter in Science, Engineering and Medicine" and "Success is What You Leave Behind" — ***Cato T. Laurencin, M.D., Ph.D.***

(100) 3D Printing Novel Methods and Applications

Monday, Nov 8, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 202

Michael Bortner, Chair
Nese Orbey, Co-Chair

Sponsored by: 3D Printing

12:30 Paper 100b: 3D Stereolithography (SLA) Printing-Based Micro-Fabrication Using Custom Polymer Resin Chemistry for Rapid Prototyping of Microfluidic Chips and Component — ***Isteaque Ahmed****, Katherine Sullivan, Aashish Priye*
12:55 Paper 100c: Mapping Process-Induced Chain Orientation in 3D Printed Parts — ***Anthony Kotula***
1:20 Paper 100d: Two-Wavelength Volumetric 3D Printing for Rapid Fabrication of Multi-Level Microfluidic Networks — ***Kaylee Smith****, Sanaz Habibi, Martin de Beer, Zachary D. Pritchard, Timothy F. Scott, Mark A. Burns*
1:45 Paper 100e: Optical Interconnects on a Flexible Substrate Utilizing Additive Manufacturing Tools — ***Roger B. Tipton****, Dianhao Hou, Thomas M. Weller, Venkat Bhethanabotla*

2:10 Paper 100f: Cold Spray of Polystyrene Particles on Various Substrates— ***Sebnem Ozbek***, *Michael J. Carter, Grant A. Crawford, Travis W. Walker*

(101) Adsorbent Materials

Monday, Nov 8, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 308

Aaron Moran, Chair
Sasidhar Gumma, Co-Chair
Federico Brandani, Co-Chair

Sponsored by: Adsorption and Ion Exchange

12:30 Paper 101b: Atmospheric Water Extraction Enabled By Smart Moisture Absorbing Foams — ***David Gamliel***, *Peter Warren, Dorin Preda, Sean Torrez, John Kidd, Cameron McConnell, Travis Emery, Caitlin Bien, Russell Lambert, Zachary Whitermore, Jacob Miske, Tiffany Yu, John Grimble, Jeffrey Yee, Bryan E. Sharkey, Todd Emrick, Ian Norris, Paul Smith*
12:50 Paper 101d: Separation of Ethylene from OCM Reaction By Cu(I)-Doped Mesoporous Carbon — ***Marisa Comroe***, *Dipendu Saha*
1:10 Paper 101f: Dual Cu(I) Active Site for CO Adsorption with Elevated Adsorption Capacity — ***Farshad Feyzbar-Khalkhali-Nejad***, *Ehsan Hassani, Ali Rashti, Tae-Sik Oh*
1:30 Paper 101g: Silver- and Copper- Immobilized-Graphene Oxide Metal Organic Frameworks for Enhanced Adsorption in Water Treatment. — ***Medha Kasula***, *Milad Esfahani, Tin Le, Adrienne Thomsen*

(102) Adsorbent Materials and Applications for Sustainable Energy and Chemicals

Monday, Nov 8, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 109

Dipendu Saha, Chair
Roger Whitley, Co-Chair
Marcus Mello, Co-Chair
Reza Haghpanah, Co-Chair

Sponsored by: Adsorption and Ion Exchange

12:30 Paper 102b: Adsorption Processes for Recovery and Enrichment of Organic Acids from Kraft Black Liquor — ***Qiang Fu***, *Meisha L. Shofner, Scott A. Sinquefield, Sankar Nair*
12:49 Paper 102c: Selective Nitrogen and Phosphorus Removal and Recovery Using Hybrid Ion Exchangers and Electro-Assisted Regeneration — ***William Tarpeh***, *Hang Dong, Brandon Clark*
1:08 Paper 102f: Metal-Organic Frameworks As a Platform to Study Impact of Surface Heterogeneity on Adsorption of Ideal Mixtures — ***Lukas Bingel***, *Krista Walton*
1:27 Paper 406b: Selective Separation of CO from CO_2 By Cu Cl Based Adsorbents — ***Maria Abbasi***, *F Handan Tezel, Kourosh Zanganeh*
1:46 Paper 406c: Development of Materials for the Direct Air Capture of CO_2Under Unconventional Conditions — ***Pranjali Priyadarshini***, *Guanhe Rim, Cornelia Rosu, Mingyu Song, Fanhe Kong, Ryan Lively, Christopher W. Jones*
2:05 Paper 406e: Carbon Dioxide Capture on Superactivated Hydrochars Derived from Loblolly Pine and Functionalized By Deep Eutectic Solvents — ***Al Ibtida Sultana***, *Toufiq Reza*
2:24 Paper 406f: Post-Synthetic Metalation of MOFs: Alternative Adsorption Sites for Sulfur Gas Uptake — ***Tania Evans***, *Krista Walton*
2:43 Paper 406h: Paraffin-Olefin Separation By Ag(I)-Doped Nanoporous Carbons: Experiment and Computation — ***Dipendu Saha***, *Giorgio DeLuca*

(103) Advancements in Particle Engineering and Material Sciences in Pharmaceutical Process Development II

Wednesday, Nov 17, 3:30 PM

Virtual, Pharmaceutical Discovery, Development and Manufacturing Forum (26)

Liang Chen, Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

3:30 Paper 360c: Deagglomeration By Conical Milling of a Temperature Sensitive Amorphous Peptide — ***Kyle Blakely***, *Kevin D. Seibert, Paul Stroud*
3:50 Paper 103e: Developing Quantitative Chemometric Models for Monitoring API Disproportionation Process with Raman Spectroscopy and X-Ray Diffraction— ***Shikhar Mohan***, *Chiajen Lai, Kevin Chu, Yi Li, Bing Shi, Liliana De La Paz*
4:10 Paper 103d: Prediction of Powder Flow of Pharmaceutical Materials from Physical Particle Properties Using Machine Learning — ***Laura Pereira Diaz***, *Cameron Brown, Ebenezer Ojo, Alastair J. Florence*
4:30 Paper 243c: A Systematic Approach to Understand Impurity Incorporation during the Crystallization of Pharmaceutical Drug Substance — ***Paridhi Agrawal***, *Saurin Hiren Rawal, Venkata Ramana Reddy, Shekhar K. Viswanath, Jeremy Merritt*
4:50 Paper 243d: Structured Approach to Optimize Pharmaceutical Crystallization Process for Optimal Impurity Rejection — ***Saurin Hiren Rawal, PhD***, *Paridhi Agrawal, Venkata Ramana Reddy, Jeremy Merritt, Shekhar K. Viswanath*
5:10 Paper 524a: Advances in Crystal Structure Prediction for Conformationally Flexible Molecules — ***Gregory Beran***
5:30 Paper 524b: How Much Do Disorder and Entropy Matter in Molecular Systems? — *Nathan Abraham, Eric Dybeck, Marcus Hock,* ***Michael Shirts***

(104) Advances in Machine Learning and Intelligent Systems I

Monday, Nov 8, 12:30 PM
Sheraton Back Bay, Independence Ballroom East

Joseph Kwon, Chair
Apoorva Sampat, Co-Chair

Sponsored by: Information Management and Intelligent Systems

12:30 Paper 104a: Design of Flow Chemistry Experiments Using Batch Bayesian Optimization — *Jose Folch,* ***Calvin Tsay***, *Mark van der Wilk, Behrang Shafei, David Walz, Astrid Niederle, Ruth Misener*
12:45 Paper 104b: Physics-Informed Machine Learning Surrogates with Optimization-Based Guarantees: Applications to AC Power Flow — *Jordan Jalving, Michael Eydenberg, Logan Blakely, Zachary Kilwein, Fani Boukouvala,* ***Carl D. Laird***
1:00 Paper 104c: Systematic Selection of Surrogate Modeling Techniques for Surrogate-Based Optimization Using Presto (Predictive REcommendations of Surrogate models To Optimize) — ***Bianca Williams***, *Selen Cremaschi*
1:15 Paper 104d: Identification of Critical Process Parameters from Observational Data, a Causal Inference Perspective — ***Shu Yang***, *B Wayne Bequette*
1:30 Paper 104e: Efficient Optimization and Accurate Approximation Using Surrogate Models – Tools and Case Studies from RAPID Synopsis Project— ***Bianca Williams***, *Sun Hye Kim, Mohammed Sadaf Monjur, Suryateja Ravutla, Fani Boukouvala, Selen Cremaschi, M M Faruque Hasan, Simon Leyland, Joannah Otashu*
1:45 Paper 104f: Data-Driven Tight Underestimation: Application to Process Safety — ***Chinmay Aras***, *Ahmed Harhara, M M Faruque Hasan*
2:00 Paper 104g: Automated Dimension Reduction with Principal Component Analysis Using Area Under Curve — ***Dhrubajit Chowdhury***, *Monique McClain, Kris Villez*
2:15 Paper 104h: Families of Data-Driven Surrogates Based on Accuracy and Complexity — ***Maaz Ahmad***, *Iftekhar Karimi*

(105) Advances in Process Control I

Monday, Nov 8, 12:30 PM
Sheraton Back Bay, Back Bay Ballroom D

Joel Paulson, Chair
Matthew Ellis, Co-Chair

Sponsored by: Systems and Process Control

12:30: Delayed Start
12:49 Paper 105b: Online Data-Gathering Lyapunov-Based Economic Model Predictive Control for Model Selection and Verification — ***Henrique Oyama***, *Helen Durand*
1:08 Paper 105c: Model Predictive Control and Observer Design for a Chemostat Reactor — ***Guilherme Ozorio Cassol Sr.***, *Stevan Dubljevic*
1:27 Paper 105d: Output Feedback Control of Nonlinear Distributed Parameter Systems with Unknown Parameters Using a Two-Tier Adaptive Identification Method — ***Davood Babaei Pourkargar***, *Antonios Armaou*
1:46: Break
2:05 Paper 105f: A Distributed Feedback Optimizing Control Framework for Large-Scale Coupled Systems with Convergence Guarantees — ***Dinesh Krishnamoorthy***
2:24 Paper 105g: Enhancing Resource Utilization Efficiency in Networked Control of Nonlinear Distributed Processes with Parametric Drift — ***Amr Zedan***,***Nael El-Farra***
2:43 Paper 105h: Application of Model Predictive Control to Wormlike Micelles Production: A Case Study of CTAB and NaCl — ***Silabrata Pahari***, *Jiyoung Moon, Sungwon Hwang, Mustafa Akbulut, Joseph Kwon*

(106) Advances in Process Design

Monday, Nov 8, 12:30 PM
Sheraton Back Bay, Independence Ballroom West

M M Faruque Hasan, Co-Chair
Salih Emre Demirel, Co-Chair
Gonzalo Guillén-Gosálbez, Co-Chair

Sponsored by: Systems and Process Design

12:30 Paper 106a: A Generalized Framework for Reactor Network Synthesis: A Graph Theoretic Approach — ***Arthur Eduardo Pastore De Lima***, *Christos Maravelias*
12:45 Paper 106b: Modeling and Performance Assessment of Rotating Packed Beds for the Production of Precipitated Carbonate Nanoparticles — ***Marianthi Dimoliani***, *Athanasios Papadopoulos, Panos Seferlis*
1:00 Paper 106c: Process Synthesis and Intensification for Shale Resources Valorization — ***Zewei Chen***, *Edwin Andres Rodriguez Gil, Rakesh Agrawal*
1:15 Paper 106d: A Short-Cut Method for Synthesis of Solvent-Based Separations — ***Shuang Xu***, *Anjan K. Tula, Selen Cremaschi, Mario Eden*
1:30 Paper 106e: Discrete-Steepest Descent: A Solution Method for Process Synthesis Generalized Disjunctive Programs — ***David Bernal***, *Daniel Ovalle, David A. Linan, Luis Ricardez-Sandoval, Jorge Gomez, Ignacio Grossmann*
1:45 Paper 106f: Optimization of Natural Gas Liquefaction Process Using Detailed Differential Algebraic Equation Based Multi-Stream Heat Exchanger Design — ***Saif R. Kazi***, *Rahul Gandhi, Lorenz Biegler*
2:00 Paper 106g: Ensuring Process Safety of Heat Exchanger Networks Under Uncertainty — ***Ahmed Harhara***, *M M Faruque Hasan*

(107) Advances in Zeolite Science and Technology I - Synthesis and Characterization (Invited Talks)

Monday, Nov 8, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 208

Thomas Degnan, Chair
Rajamani Gounder, Co-Chair

Sponsored by: Advances in Zeolite Science and Technology

12:30 Paper 107b: Insights into Structural Details of Zeolites Via Three-Dimensional Electron Diffraction — ***Zhehao Huang***
12:55 Paper 107c: Synthetic and Post-Synthetic Methods to Alter Al-Al Site Pair Arrangements in Zeolites — ***Songhyun Lee***, *Elizabeth Bickel, Claire Nimlos, David Hibbitts, William Schneider, Rajamani Gounder*
1:15: Break
1:45 Paper 107e: Hydrogen Bonding in Zeolites in Acid Sites and Defects— ***Hubert Koller***, *Christian Schroeder, Michael R. Hansen, Michael Hunger, Christopher M. Lew, Stacey Zones*
2:15 Paper 461e: Correlating Nanoscale Compositions, Structures, and Reaction Properties of Bifunctional Pt-H^+usy Zeolite Catalysts — ***Tsatsral Battsengel***, *Michael Girgis, Stacey Zones, Bradley F. Chmelka*
2:35 Paper 229b: Mechanistic Role of Water in the Storage and Oxidation of NO on Pd/CHA — ***Surya Pratap Solanki***, *Mugdha Ambast, Christopher Paolucci, Michael Harold, Lars Grabow*

(108) Applications of Data Science to High Throughput Experimentation

Monday, Nov 8, 12:30 PM
Marriott Copley Place, Salon H/I

Elizabeth Nance, Chair
Johannes Hachmann, Co-Chair

Sponsored by: Applications of Data Science to Molecules and Materials

12:30 Paper 108a: Virtual High-Throughput Screening of Vapor-Deposited Amphiphilic Polymers for Biofilm Reduction with Machine/Deep Learning— ***Zhihao Feng***, *Yifan Cheng, Andrew L. Hook, Rong Yang, Jeffrey D. Varner*
12:45 Paper 108b: High-Throughput and Data-Driven Strategies for the Design of Deep Eutectic Solvent Electrolytes. — ***Jaime Rodriguez Jr.***, *Maria Politi, Lilo Pozzo*
1:00: Break
1:15 Paper 108d: AI-Guided Autonomous Flow Reactor Platform for Accelerated Nanomaterial Synthesis Screening and Parameter Space Mapping— *Ajit Vikram, Arwa Zahid,* ***Paul Kenis***
1:30 Paper 108e: Machine Learning Models for Rapid Compositional Quantification of Complex Multicomponent Mixtures Using Vibrational Spectroscopy — ***Andrea Angulo Figueira***, *Lankun Yang, Eray Aydil, Miguel Modestino*
1:45 Paper 108f: Are Structure-Function Relationships Governing Polymeric Gene Delivery Payload-Specific? — ***Ramya Kumar***, *Ngoc Le, Mary Brown, Theresa M. Reineke*
2:00 Paper 108g: Enhancing Insight to Individual and Population-Based Microglial Reactivity with Image Analysis — ***Hawley Helmbrecht***, *Elizabeth Nance*
2:15 Paper 108h: High-Affinity Non-Immunoglobin Scaffolds Promoted By Sequence Mining Impactful in High-Value Therapeutics — ***Mehrsa Mardikoraem***, *Joelle Eaves, Daniel Woldring*
2:30 Paper 108i: Intelligent Molecular Surgery Platform Via Reinforcement Learning — ***Jiali Li***, *Jie Su, Zhiyao Luo, Jiahao Wang, Yixin Zhu, Xiaonan Wang, Jiong Lu*

(109) Applied Artificial Intelligence, Big Data, and Data Analytics Methods for Next-Gen Manufacturing Efficiency I

Monday, Nov 8, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 201

Joel Paulson, Chair
Mona Bavarian, Co-Chair

Sponsored by: Next-Gen Manufacturing

12:30 Paper 109a: Use of Dimensionality Reduction and Transfer Learning in Deep Reinforcement Learning Controller for Hydraulic Fracturing— ***Mohammed Saad Faizan Bangi***, *Joseph Kwon*
12:50 Paper 109b: Harnessing Cognitive AI Technology in Refining to Enhance Operator Decisions — ***Leslie Rittenberg***
1:10 Paper 109c: Regression Model for Tool Wear Monitoring in Precision Machining — ***Seulki Han***, *Nasir Mannan, George Bollas*
1:30 Paper 109d: Selection of Combined Index Weights to Optimize Anomaly Detection in Big Area Additive Manufacturing — ***Monique McClain***, *Dhrubajit Chowdhury, Kris Villez*
1:50 Paper 109e: Keynote Talk - Topological Data Analysis: Concepts, Computation, and Applications in Manufacturing — *Alexander Smith,* ***Victor Zavala***
2:25 Paper 109f: Keynote Talk - Platforms and Algorithms for Digitally-Enabled Next-Gen Manufacturing — ***R Donald Bartusiak***, *Thomas Badgwell, John B. Vicente*

(110) Area Plenary: Leaders in Biomaterials (Invited Talks)

Monday, Nov 8, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 103

Julianne Holloway, Chair
Matthew Webber, Co-Chair
Catherine Fromen, Co-Chair

Sponsored by: Biomaterials

12:30 Paper 110a: Shuttling Nanoparticles to the Vascular Wall Via Deformable, Vascular-Targeted Microparticles — ***Lola Eniola-Adefeso***
1:20 Paper 110b: Biomaterial-Mediated Immunotherapeutic Drug Delivery to Lymph Nodes Augments Cancer Immunotherapy — ***Susan Thomas***
2:10 Paper 110c: Regulating Lipid Metabolism and Inflammation Resolution Pathways Using Engineered Materials — ***Edward Botchwey***

(111) Biomass Upgrading I: Reaction Fundamentals

Monday, Nov 8, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 207

Juan Bravo-Suarez, Chair
Yang Xiao, Co-Chair
Canan Sener, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

12:30 Paper 111c: Mechanistic Investigation into the Formation of Humins in Acid Catalyzed Liquid Phase Biomass Reactions. — ***Jose Carlos Calderon***, *Samir H. Mushrif, Jyotsna S. Arora*
12:48 Paper 111d: Determining the Adsorption Energetics of 2,3-Butanediol on RuO_2(110) from First Principles — ***Carrington Moore***, *Difan Zhang, Roger Rousseau, Vassiliki-Alexandra Glezakou, Jean-Sabin McEwen*
1:06 Paper 111e: Upgrading Erythrose over Lewis Acidic Metal Oxides — ***Sean Najmi***, *Andrew Medford, Carsten Sievers*
1:24 Paper 111f: A Scalable Synthesis of Dimethyl 2,2'-Bifuran-5,5'-Dicarboxylate Via the Oxidative Coupling of 2-Methyl Furoate — ***Mingchun Ye***, *Raul Lobo*
1:42 Paper 111g: Kinetics Study of the Hydrodeoxygenation of Xylitol over a ReO_x-Pd/CeO_2 Catalyst — ***Blake MacQueen***, *Michael Royko, Bradie S Crandall, Andreas Heyden, Yomaira J. Pagan-Torres, Jochen Lauterbach*
2:00 Paper 111h: Investigating Thermodynamics and Kinetics of the Formation of Lignin-Carbohydrate Complex Linkages in Lignocellulosic Biomass Using *Ab Initio* Methods — ***Seth Beck***, *Samir H. Mushrif, Phillip Choi*
2:18 Paper 53a: Kinetic Analysis and Reaction Mechanism for Pentanoic Acid Conversion over Promoted Molybdenum Oxide — ***Laura Alejandra Gomez Gomez***, *Reda Bababrik, Steven Crossley*
2:36 Paper 53h: Capturing the Coverage Dependence of Aromatics Via Mean-Field Models: Application in the Hydrodeoxygenation of Biofuels — ***Naseeha Cardwell***, *Alyssa Hensley, Yong Wang, Jean-Sabin McEwen*

(112) Biomolecules at Interfaces

Monday, Nov 8, 12:30 PM
Sheraton Back Bay, Back Bay Ballroom A

Roberto Andresen Eguiluz, Chair
Younjin Min, Co-Chair
Prajnaparamita Dhar, Co-Chair

Sponsored by: Interfacial Phenomena

12:30 Paper 112a: Phosphate Recovery By a Surface-Immobilized Cerium Affinity Peptide — ***Zihang Su***, *Jacob Hostert, Julie Renner*
12:45 Paper 112b: Self-Assembly and Rearrangement of a Polyproline II Helix Peptide on Gold — ***Jacob Hostert***, *Charles Loney, Nuttanit Pramounmat, Katherine Yan, Zihang Su, Julie N. Renner*
1:00 Paper 112c: Interactions between DNA-Functionalized Carbon Nanotubes and Proteins in Solution — ***Rebecca Pinals***, *Clayton Radke, Markita Landry*
1:15 Paper 112d: Intermolecular Interactions of λ-Carrageenan with Phytanic Acid and Ca^{++} at the Air-Water Interface Using X-Ray Reflectivity — ***Luis Ortuno Macias***, *Hao Zhou, Ankit Kanthe, Charles Maldarelli*
1:30 Paper 112e: Protein Adsorption and Corona Formation on Silica Nanoparticles: Effect of pH and Electrolyte — ***Jin Gyun Lee***, *Bhuvnesh Bharti*
1:45 Paper 112f: Self-Assembling Cellular Coatings to Improve the Oxygen Tolerance of Anaerobes — ***Gang Fan***, *Ariel Furst*
2:00 Paper 112g: Thin-Layer Rheology of Biological Lipid/Lipoprotein Surfactants Using Quartz-Crystal Microbalance with Dissipation — ***Bernardo Yanez Soto***, *Silvia Jonguitud-Flores, Gabriel Espinosa-Pérez, Maxim Yutkin, Clayton Radke*
2:15 Paper 112h: Relating Interfacial Morphology, Curvature, and Dilatational Modulus for Surfactant Films — ***Steven Iasella***, *Sourav Barman, Clara Ciutara, Joseph Zasadzinski*
2:30 Paper 112j: Reagentless Modification of Surfaces with Biomolecules— ***Ariel Furst***

(114) Carbon Nanomaterials: Graduate Student Award Session

Monday, Nov 8, 12:30 PM
Marriott Copley Place, Wellesley

Anju Gupta, Chair
Xiaoxue Wang, Co-Chair
Rebecca Pinals, Co-Chair

Sponsored by: Carbon Nanomaterials

12:30 Paper 114a: Data Management Schema Design for Effective Nanoparticle Formulation for Probing and Treating Neurological Disease — ***Hawley Helmbrecht***, *Andrea Joseph, Rick Liao, Nuo Xu, Chih-Chung Chen, Elizabeth Nance*
12:45 Paper 114b: Stimuli Responsive Self-Folding 3D Graphene Architectures— ***Qi Huang***, *Tao Deng, Weinan Xu, ChangKyu Yoon, Zhao Qin, Yida Lin, Tengfei Li, Yuqian Yang, Libin Yang, Susanna Thon, Jacob B. Khurgin, David Gracias*
1:00 Paper 206f: Rheoelectric Characterization of Oxidized Carbon Nanoparticles As Slurry Active Materials — ***Paolo Ramos***, *Connor Call, Lauren Simitz, Jeffrey Richards*
1:15 Paper 114d: Controllable Synthesis of Hybrid Nanocomposite Structures *Via* Laser Ablation Technique for Electrochemical Energy Storage and Conversion Devices — ***Mahshid Mokhtarnejad***, *Erick L. Ribeiro, Dibyendu Mukherjee, Bamin Khomami*
1:30 Paper 114e: Fundamental Process Parameters and Fiber Formation Mechanisms in Wet-Spinning of

Carbon Nanotube Fibers — ***Oliver Dewey***, *Lauren Taylor, Samantha Fowler, Glen Irvin, Matteo Pasquali*
1:45 Paper 114f: Investigating the Mechanism of Temperature-Induced Graphene Self-Folding in Water — ***Soumil Joshi***, *Samrendra Singh, Karteek K. Bejagam, Sanket Deshmukh*
2:00 Paper 114g: Utilizing Unique Thermodynamic Equilibria of Co-Surfactant States Around Nanotubes for Optical Biosensors — ***Aniruddha Kulkarni***, *Stephen Michel, Yang Zhao, Kirk J. Ziegler*
3:30 Paper 114h: Gold Nanoparticles Deposited inside Hierarchical Zeolites Catalyze Diverse Groups of Aromatic Alcohols — ***Zengran Sun***, *Steven Saunders*

(115) Cellular and Biochemical Sensing Technologies

Monday, Nov 8, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 110

Maryam Raeeszadeh Sarmazdeh, Chair
Shachi Mittal, Co-Chair

Sponsored by: Bioengineering

12:30 Paper 115a: Programming Cell-Free Biosensors with DNA Strand Displacement Circuits — ***Jaeyoung Jung***, *Khalid K. Alam, Julius B. Lucks*
12:51 Paper 115b: Label-Free Optical Electrophysiology Using Electrochromic Materials — ***Yuecheng Peter Zhou***, *Erica Liu, Holger Muller, Bianxiao Cui*
1:12 Paper 115c: Diffusion of High Concentrations of Unlabeled IgG and BSA in a Hydrophilic, Hyaluronic Acid Gel — ***Antonio Dos Santos***, *Eduardo Ximenes, Casey Bomrad, Jorge Martinez, Jessica Zuponcic, Adib Ahmadzadegan, Arezoo Ardekani, Pavlos Vlachos, Michael Ladisch, Shiven Kapur, Vincent Corvari*
1:33 Paper 115d: Engineering the *P*-Coumaric Acid Responsive Biosensor System Padr-P_{padC} for Versatile Dynamic Properties — ***Tian Jiang***, *Chenyi Li, Yajun Yan*
1:54 Paper 115e: Multiplexed Live Cell Imaging Using Ultra-Fast Cycling— ***Jina Ko***, *Evangelia Bolli, Mikael Pittet, Ralph Weissleder, Jonathan Carlson*
2:15 Paper 115f: Test for Sickle Cell Disease Vaso-Occlusive Crisis Using Cell Tracking Velocimetry — ***Mitchell Weigand***, *Jeffrey Chalmers, Jenifer Gómez-Pastora*
2:36 Paper 115g: Programming STAND Displacement Circuits for Dynamic Protein Assembly and Biosensing — ***Wilfred Chen***

(116) Chemical Recycling of Waste Plastics II

Monday, Nov 8, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 205

Wan-Ting Chen, Chair
Sheima Khatib, Co-Chair
Hilal Ezgi Toraman, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

12:30 Paper 116a: Plastic Polypropylene to Lubricants Using Hydrogenolysis— ***Pavel Kots***, *Brandon Vance, Dionisios Vlachos*
12:50 Paper 116b: Selective Hydrogenolysis of Polyethylene and Polypropylene to Liquid Alkanes over Tunable Ruthenium-Based Heterogeneous Catalysts— ***Julie Rorrer***, *Gregg T. Beckham, Yuriy Roman*
1:10 Paper 116c: Effect of Chain Branching on the Hydrogenolysis of Heptane Isomers over Metal Catalysts: Insights to Hydrogenolysis of Polyethylene.— ***Olajide Bamidele***, *Andreas Heyden*
1:30 Paper 116d: Chemical Upcycling of Polyethylene Using Heterogeneous Alkane Cross-Metathesis — ***Doyoung Kim***, *Raul Lobo*
1:50 Paper 116e: Selective Production of Gasoline Range Iso-Alkanes from Polyolefin Plastics — ***Changle Jiang***, *Yuxin Wang, Thang Luong, Brandon Robinson, Jianli Hu*
2:10 Paper 116f: Bridging the Gap between Model Alkanes and Polyethylene Waste Hydrocracking — ***Brandon Vance***, *Pavel Kots, Dionisios Vlachos*

(117) Continuous Drug Substance – Integrated Processes - Session 2

Monday, Nov 8, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 102

Nicholas Vecchiarello, Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

12:30 Paper 117a: Continuous Manufacturing of Beta-Lactam Antibiotics By Enzymatic Synthesis and Crystallization: A Pilot Plant Study — ***Hossein Salami***, *Patrick Harris, Colton Lagerman, Matthew McDonald, Ronald Rousseau, Martha Grover, Andreas Bommarius*
12:54 Paper 58b: Development of a Stable and Recyclable Biocatalyst for the Reactive Crystallization of Cephalexin Monohydrate — ***Patrick Harris***, *Hossein Salami, Ronald Rousseau, Martha Grover, Andreas Bommarius*
1:18 Paper 117b: Adaptation of a Small-Scale Additive Manufacturing System to Enable End to End Continuous Production of Solid Oral Drug Products — ***Varun Sundarkumar***, *Zoltan Nagy, Gintaras V. Reklaitis*
1:42 Paper 117c: Intensified Continuous Purification Platform for Pharmaceutical Systems - Application to the Continuous Manufacturing of Pure Cannabidiol Crystals — ***Inyoung Hur***, *Wei-Lee Wu, Ayse Eren, Jaron Mackey, Rojan Pavaresh, Zoltan Nagy*
2:06 Paper 117e: Real Time Process Monitoring with PAT for Continuous Pharmaceutical Manufacturing: Toward Advanced Process Control and Real Time Optimization with Ciprofloxacin Synthesis — ***Yuma Miyai***, *Anna Forzano, Cameron Armstrong, Luke Rogers, Thomas Roper*
2:30 Paper 117f: Dynamic Flowsheet Simulation and Application of Soft Sensors on an Intensified and Integrated Purification Step for Pharmaceutical Upstream Manufacturing — ***Inyoung Hur***, *Daniel Casas-Orozco, Zoltan Nagy*

(118) Data-Driven Design and Modeling I

Monday, Nov 8, 12:30 PM
Marriott Copley Place, Salon J/K

Stephanie Valleau, Chair
Yi He, Co-Chair
Qing Shao, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

12:30 Paper 118a: The Machine Learning Route to Accelerated Discovery and Inverse Design of Chemical and Materials Systems — ***Johannes Hachmann***
1:00 Paper 118b: A Universal Framework for Featurization of Atomistic Systems— ***Andrew Medford***, *Ray Lei*
1:15 Paper 118c: Transfer Learning Using Large-Scale ML Models for Catalyst/Molecular Datasets — ***Adeesh Kolluru***, *Muhammed Shuaibi, Zachary Ulissi*
1:30 Paper 118d: Semi-Supervised Learning Detects Safe Islands Where Density Functional Theory Is Applicable for Chemical Discovery — ***Chenru Duan***, *Aditya Nandy, Fang Liu, Heather Kulik*
1:45 Paper 118e: *In silico* discovery of Target Peptide Inhibitors for *C. Diff* toxins a and B — ***Sudeep Sarma***, *Xingqing Xiao, Stefano Menegatti, Nathan Crook, Scott Magness, Carol Hall*
2:00 Paper 118f: You May Not Have Noticed, but Your Neural Network Did: Machine Learning from Simulated Enzyme Variants — ***Tucker Burgin***, *David Beck, Jim Pfaendtner*
2:15 Paper 118g: Deep Reinforcement Machine Learning Driven Vaccine Design Against Highly Mutable Pathogens — ***Jonathan Faris***, *Brenden Peterson, Daniel Faissol, Kayla Sprenger*
2:30 Paper 118h: Data-Driven Reconstruction of Molecular Folding Trajectories from Single-Molecule Experimental Measurements — ***Maximilian Topel***, *Andrew Ferguson*
2:45 Paper 118i: High-Throughput Screening of Tribological Properties of Monolayer Films Using Molecular Dynamics and Machine Learning — ***Co D. Quach***, *Justin Gilmer, Christopher Iacovella, Peter Cummings, Clare McCabe*

(119) Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains II

Monday, Nov 8, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 313

Dharik Mallapragada, Chair
Christos Maravelias, Co-Chair
Arpa Ghosh, Co-Chair

Sponsored by: Sustainable Energy

12:30 Paper 119a: Capturing Spatial, Temporal and Technological Detail in Hydrogen Supply Chains By a Bilevel Optimization Strategy — *Victor Cantu Medrano, Eduardo Carrera, Antonin Ponsich,* ***Catherine Azzaro-Pantel***
12:55 Paper 119b: Exploring the Distributional Impacts of Heat Decarbonisation: A Cost-Benefit Analysis and Whole-System Optimisation of the UK Heating System — ***Jennifer Penman***, *Sheila Samsatli*
1:20 Paper 119c: Spatially-Explicit Techno-Ecological Design for Sustainable Manufacturing and Minimized Air Pollution Health Impacts — ***Michael Charles***, *Bhavik Bakshi*
1:45 Paper 119d: Decision Tree-Based Optimisation for Flexible Energy Storage Dispatch — *Liam Kirkby, Diarmid Roberts,* ***Jude O. Ejeh***, *Solomon F. Brown*
2:10 Paper 119e: Tracking Embodied Co, Li, Mn, and Ni Material Flows in the US through Economic Input-Output-Based Network Analysis — ***Miriam Stevens***, *Shweta Singh, Sarang Supekar*

(120) Design for a Circular Economy-I

Monday, Nov 8, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 311

William Barrett, Chair
Konstantinos E. Kakosimos, Co-Chair
Shweta Singh, Co-Chair

Sponsored by: Sustainability Science and Engineering

12:30 Paper 120b: Dynamic Material Flow Analysis of Crystalline Silicon Solar Cells for Circular Economy Transition — ***Sherif Khalifa***, *Benjamin V. Mastrorocco, Dylan D. Au, Teresa M. Barnes, Alberta Carpenter, Jason Baxter*
12:55 Paper 120c: Developing Innovation Roadmaps for Plastics Value-Chain Using Sustainable Circular Economy Framework — ***Vyom Thakker***, *Fatima Hafsa, Terrence Wilson, Kevin Dooley, Bhavik Bakshi*
1:20 Paper 120d: Systems Analysis Approach to PET and Olefin Plastics Supply Chains in the Circular Economy — ***Utkarsh Chaudhari***, *Yingqian Lin, Vicki Thompson, Robert Handler, Joshua Pearce, Gerard Caneba, Prapti Muhuri, David W. Watkins, David Shonnard*
1:45 Paper 120e: Micron: A Quantitative, Holistic and Robust Circular Economy Assessment Framework at the Micro Level — ***Stefanos Baratsas***, *Efstratios N. Pistikopoulos, Styliani Avraamidou*
2:10 Paper 120f: Integrated Framework for the Design of Intensive Cattle and Agricultural Operations Towards Circular Economy. — *Manuel Taifouris,* ***Mariano Martin***

(121) Developments in Alternative Fuels and Enabling Technologies

Monday, Nov 8, 12:30 PM
Marriott Copley Place, Fairfield

Ashwin Ravichandran, Chair

Keyvan Mollaeian, Co-Chair

Sponsored by: Fuels and Petrochemicals Division

12:30 Paper 121a: Simulation Study of Chemical Transesterification Reaction for Biodiesel Production from Castor Oil — *Sakib Nehal, Ashib Anzum,* ***Md. Iqbal Hossain***
12:47 Paper 60a: Meeting U.S. Liquid Fuel Requirements Using Biomass Feedstocks to Replace Crude Oil in Large Integrated Refineries — ***Charles Forsberg****, Bruce Dale*
1:04: Break
1:21 Paper 121d: Synthesis of Renewable Jet Fuel Range Cycloparaffins with Levulinic and Formic Acids — ***Sampath Karunarathne****, Matthew J. Kline, Scott Eaton, Hemant P. Pendse, M Clayton Wheeler*
1:38 Paper 121e: Sustainable Aviation Fuel from Waste Streams— ***Karthikeyan Ramasamy****, Mond Guo, Senthil Subramaniam, Lesley Snowden-Swan, Casper Brady, Chirag Mevawala*
1:55: Break
2:12 Paper 121g: Influence of Alcohol Additives on the Viscosity and Solubility of Ethanol/Diesel Fuel Blends: A Molecular Dynamics Simulation Study— ***Xueying Li****, Lei Hou, Chong Chai, Sichen He*

(122) Dynamic Processes in Polymer Networks and Gels

Monday, Nov 8, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 104

Nese Orbey, Chair
Jinhye Bae, Co-Chair
Monirosadat Sadati, Co-Chair

Sponsored by: Polymers

12:30 Paper 122a: Structural Control of Resorcinol-Formaldehyde Xerogels and Their Subsequent Processing into Magnetic Carbon Rods — ***Joelle Medinger****, Marco Lattuada*
12:45 Paper 122b: Hydrogels Equipped with an 'On-Off Switch' for Solute Release — ***Sai Nikhil Subraveti****, Srinivasa R. Raghavan*
1:00 Paper 122c: Stimuli Responsive Reversible Adhesion between Physical and Chemical Networks — ***Leah K Borden****, Srinivasa R. Raghavan*
1:15 Paper 122d: Examining the Initial Curing Mechanism of Ethyl Linoleate Using Monomer-Based Kinetic Monte Carlo Simulation — ***Rebecca Harmon****, Piet Iedema, Linda Broadbelt*
1:30 Paper 122e: Effect of Interdroplet Interactions on Pore Interconnectivity of Polymerized High Internal Phase Emulsions — ***Muchu Zhou****, Alireza Bandegi, Reza Foudazi*
1:45 Paper 122f: Dynamics of Reversible Phase Transition of Thermo-Responsive Natural Polymers — ***Navid Bizmark****, Nicholas J. Caggiano, Jason X. Liu, Craig B. Arnold, Robert K. Prud'homme, Sujit Datta, Rodney Priestley*
2:00 Paper 122g: Hybrid Hydrogels Comprising Interpenetrating Electrostatic and Covalent Networks — ***Defu LI****, Tobias Gockler, Samanvaya Srivastava*
2:15 Paper 122h: High Charge Density Interpenetrating Hydrogels of Hydrolyzed Networks of Poly(N-Vinyl Formamide) and Polyacrylamide— ***Joseph Scalet****, Tiffany C. Suekama, Jeayoung Jeong, Stevin Gehrke*
2:30 Paper 122i: Investigating the Mechanical and Transport Properties of Thermally- and Chemically-Crosslinked Poly(vinyl alcohol)–Lignin Soft Composites — ***Nicholas Gregorich****, Graham Tindall, Sagar Kanhere, Jaden Stutts, Tyler Martin, Amod Ogale, Mark Thies, Eric M. Davis*
2:45 Paper 122j: Phase-Separation, Gelation, and Dynamics of Associative Polymers — ***Scott Danielsen, PhD****, Michael Rubinstein*

(123) Electrocatalysis and Photoelectrocatalysis III: Organic Electrocatalysis

Monday, Nov 8, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 203

Miguel Modestino, Chair
Maureen Tang, Co-Chair
Ramchandra Gawas, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

12:30: Break
12:48 Paper 123b: Understanding CO and Methanol Electro-Oxidation Activity on Ag_xPd_{1-x}/C Alloys Under Alkaline Conditions — ***Adam Baz****, Taylor Spivey, Adam Holewinski, Lindsey Hamblin*
1:06 Paper 123c: Influence of an External Potential on the Solvation Thermodynamics of Intermediates in the Pathway for Methanol Oxidation on Pt(111) — ***Ali Estejab****, Rachel Getman*
1:24 Paper 123e: Chlorine-Mediated Electrochemical Ethylene Oxidation in Saline Water — ***Minju Chung****, Kyoungsuk Jin, Joy Zeng, Karthish Manthiram*
1:42 Paper 123f: Electrochemical Biomass Upgrading: Degradation of Glucose to Lactic Acid on a Copper (II) Electrode — ***Lars Ostervold III****, Sergio I. Perez Bakovic, Jamie Hestekin, Michael Janik, Lauren F. Greenlee*
2:00 Paper 123g: Electrochemical C(sp^3)-H Bond Oxidation of Xenobiotics with Mediators — ***Mayank Tanwar****, Sagar Udyavara, Masato Saito, Yu Kawamata, Matthew Sigman, Shelley Minteer, Phil Baran, Matthew Neurock*
2:18 Paper 123h: Competing Kinetics between Electrochemical Reduction of Furfural and Non-Electrochemical Homogeneous Side Reactions — *Andrew May, Steven Watt,* ***Elizabeth Biddinger***

(124) Electrochemical CO2 Conversion II

Monday, Nov 8, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 206

Carlos Morales-Guio, Chair
Jeremy T. Feaster, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

12:30 Paper 124a: The Electrochemical Kinetics of Hydrocarbon Synthesis from CO_2: A Unified Picture of Surface Intermediates and Their Interaction with Electrolyte Ions — ***Marcel Schreier***
12:48 Paper 124b: Mass Transport Controls Product Selectivity in Electrocatalytic CO_2 Reduction on Copper — ***Joonbaek Jang****, Carlos Morales-Guio*
1:06 Paper 124c: Operando Attenuated Total Reflection Surface Enhanced Infrared Spectroscopy of the Electrochemical CO_2 Reduction Reaction on Gold Thin Films Under Mass Transport Control — ***Jaime Aviles Acosta****, John Lin, Thomas Jaramillo, Christopher Hahn*
1:24 Paper 124d: The Role of Surface Roughening in Improving the Selectivity of Copper for CO2 Electroreduction — ***Joseph Gauthier****, Joakim Halldin Stenlid, PhD, Frank Abild-Pedersen, Martin Head-Gordon, Alexis Bell*
1:42 Paper 124e: The Role of Anion Exchange Membrane in CO Electroreduction — ***Bjorn Hasa****, Sean Overa, Feng Jiao*
2:00: Break
2:18 Paper 67h: Advanced Manufacturing for Electrosynthesis of Fuels and Chemicals from CO_2 — ***Jeremy T. Feaster****, Daniel Corral, Sadaf Sobhani, Joshua R. DeOtte, Dong Un (Daniel) Lee, Andrew Wong, Julie Hamilton, Victor Beck, Amitava Sarkar, Christopher Hahn, Thomas Jaramillo, Sarah Baker, Eric B. Duoss*
2:36 Paper 124h: Macroscale Modeling of Electrochemical CO_2 Reduction on Copper Catalysts — ***Justin Bui****, Lien-Chun Weng, Kaitlin Rae M. Corpus, Adam Weber, Alexis Bell*

(125) Emerging Topics in Electrochemical Engineering: Electrochemical Separations (Invited Talks)

Monday, Nov 8, 12:30 PM
Sheraton Back Bay, Commonwealth

Christopher Arges, Chair
William Tarpeh, Co-Chair

Sponsored by: Electrochemical Fundamentals

12:30 Paper 125a: Concentration Dependence of Ion Exchange Membrane Permselectivity: Modelling and Experimental Validation — ***Orlando Coronell***
1:05 Paper 125b: Molecular Design of Electroactive Redox-Interfaces for Integrating Separations and Reactions — ***Xiao Su***
1:40 Paper 125c: Direct Electrochemical Reduction to Separate Selenium from Industrially Impacted Water — ***Shiqiang Zou****, Meagan Mauter*

(126) Environmental Division Awards and Honors (Invited Talks)

Monday, Nov 8, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 309

Kristina Wagstrom, Chair

Sponsored by: Environmental Division

12:30 Paper 126a: Use of Environmental Sustainability Principles to Help Solve Environmental Problems of Concern Today — ***Robert Peters***
1:15 Paper 126b: Advancing Methodologies for Sustainability assessment of transition to Low Carbon and Circular Economy via integration of process systems engineering and macroeconomics — ***Shweta Singh***
1:45: Presentation of Student Paper Awards

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

Monday, Nov 8, 12:30 PM
Marriott Copley Place, Salon A/B

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

Sponsored by: Thermodynamics and Transport Properties

12:30 Paper 127a: Fast Single-Sequence Protein Structure Prediction with Applications in Protein Design and Novel Biomaterials — ***Ratul Chowdhury***
12:42 Paper 127b: The Search for Novel Mesoscale Materials — ***Rose Cersonsky***
12:54 Paper 127c: Dynamics of Complex Fluids and Soft Materials— ***Abhinendra Singh***
1:06 Paper 127d: A Predictive Multi-Scale Computational Model for Protein-Functioned Reversible Silica Nanoparticle Self-Assembly — ***Xin Qi****, Jaehun Chun, Christopher J. Mundy, Jim Pfaendtner*
1:18 Paper 127e: Reconfigurable Colloidal Assemblies Via Active Matter Coupled to Defects — ***Bryan VanSaders****, Sharon C. Glotzer*
1:30 Paper 127f: Evaporative Templating for Directing Hierarchical, Multi-Component Nanoparticle Assemblies — ***Thi Vo****, Katherine Elbert, Sharon Glotzer, Christopher B. Murray*
1:42 Paper 127g: Crystal-Phase Polymorphism in Nanoplates Via Competition between Energy and Entropy — ***Timothy C. Moore****, Joshua Anderson, Ronald LaCour II, Sharon C. Glotzer*
1:54 Paper 127h: Plasmonic Coupling in Self-Assembled Nanocrystal Gels and Superlattices — ***Zachary Sherman****, Manuel Dominguez, Jiho Kang, Stephen Gibbs, Kihoon Kim, Delia Milliron, Thomas Truskett*
2:06 Paper 127i: Relating Energy Dissipation to Effective Interactions and Structure Formation in Cross-Linked Biopolymer with Molecular Motors — *Alexandra Lamtyugina,* ***Yuqing Qiu****, Aaron Dinner, Suriyanarayanan Vaikuntanathan*

2:18 Paper 127j: Simulating Chemically Fueled Molecular Motors — ***Alex Albaugh***, *Todd Gingrich*
2:30 Paper 127k: Multiscale Modeling of Hierarchical Nanomaterials Via Molecular and Colloidal Self-Assembly — ***Mingfei Zhao***

(128) Flexible Platforms for Investigating Cellular Processes

Monday, Nov 8, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 108

Jonathan Soucy, Co-Chair
Adriana San Miguel, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

12:30 Paper 128a: High-Throughput DNA-Directed Patterning As a Tool to Study Prostate Cancer-Bone Marrow Niche Interactions at Single Cell and System Level — ***Molly Kozminsky***, *Lydia L. Sohn*
12:48 Paper 128b: Straightforward Incorporation of Tailorable Stromal Compartments into Microfluidic Microphysiological Systems — ***Katherine Nelson***, *Daniel J. Minahan Jr., Sarah A. Geissler, Jason P. Gleghorn*
1:06 Paper 128c: Multi-Sensor Integration into Multi-Layer Organ-on-Chip— ***Ryan Brady***, *Adam J. Bindas, Erika Wheeler, Ryan Koppes, Abigail Koppes*
1:24 Paper 128d: A Microfluidic Approach to Detect Heterogenous Alkaline Phosphatase Activity in Single *Chlamydomonas Reinhardtii* Cells — ***Alireza Rahnama***, *Manibarathi Vaithiyanathan, Adam Melvin*
1:42 Paper 128e: In Vitro Generation of Red Blood Cell Extracellular Vesicles (REVs) and Functional Evaluation of REV-Mediated Acute Endothelial Activation in Individual Patients with Genetic Hemoglobin Disorders — ***Ran An***, *Umut Gurkan*
2:00 Paper 128f: A Novel Microfluidic Device for Investigating the Long-Term Effects of Confinement on Cell Phenotype and Function — ***Farnaz Hemmati***, *Ayuba Akinpelu, Farshad Amiri, Panagiotis Mistriotis*
2:18 Paper 128g: Make Microfluidics Work for Omic Assays (Invited Speaker)— ***Chang Lu***

(129) Fluidization: Experimental and Modeling Investigation of Fluidization Processes & Circulating Fluidized Beds

Monday, Nov 8, 12:30 PM
Sheraton Back Bay, Fairfax A/B

Lev Davydov, Chair
Bodhisattwa Chaudhuri, Co-Chair
Shyam Sundaram, Co-Chair
Christopher M. Boyce, Co-Chair

Sponsored by: Fluidization and Fluid-Particle Systems

12:30: Break
12:49 Paper 129b: An Experimental Investigation of Ultra-High Temperature and Pressure Fluidized Bed for Thermal Energy Storage and Transfer — ***Jason Schirck***, *Zhiwen Ma, Aaron Morris*
1:08 Paper 701c: A Modified Frictional Solids Stress Model Fortwo Fluid Modeling of Gas-Solid Fluidized Beds — ***Qiang Guo***, *Christopher M. Boyce*
1:27 Paper 129d: The Effects of Adding Soft Particles on the Clogging of Rigid Particles in a 2D Hopper — ***Saeed Alborzi***, *Sara Hashmi*
1:46 Paper 129e: CFD Simulation of the Entire Circulating Fluidized Bed (CFB) Carbon Capture Loop Using Solid Supported Amine Sorbents — ***Farnaz Esmaeili Rad***, *Javad Abbasian, Hamid Arastoopour*
2:05 Paper 129f: Computational Modeling for FCC RTD Design Optimization— ***Raj Singh***, *Steve Shimoda*

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

Monday, Nov 8, 12:30 PM
Sheraton Back Bay, Liberty B/C

Katie Cadwell, Chair
Stephen Thiel, Co-Chair
Troy Vogel, Co-Chair

Sponsored by: Undergraduate Education

12:30 Paper 130a: Teaching How to Fish: Mentoring Students in Job/Internship Networking — ***Brad Bundy***
12:50 Paper 130b: Teaching Technical Writing to Chemical Engineers— ***George Prpich***
1:10 Paper 130c: A Spectrum of Beliefs: A Study of Undergraduate Learning Assistant Reflections As Novice Teachers — *Brandon Jeong,* ***Harpreet Auby***, *Milo Koretsky*
1:30 Paper 130d: Using Virtual Learning Communities for Remote Learning in Large Lecture-Based and Flipped Classrooms. — ***Stephanie Velegol***, *Stephanie Velegol*
1:50: Break
2:00 Paper 130e: Design and Analysis of a Sars-Cov-2 Vaccine Facility in a Remote Learning Format — ***Benjamin Davis***, *Jennifer Weiser, Ogbannaya Okorafor*
2:20 Paper 130f: Products from Pandemic Labs: Custom at-Home & Benchtop Unit Operations Teaching Modules — ***Anthony Butterfield***, *Thang Tran, Ignacio Preciado, Geoffrey Silcox, Eric Eddings, Andrew Simonson*
2:40 Paper 130g: Taking Cheme-Sports from on-Site to a Live Virtual Competition — ***Robert Bozic***, ***Matthew B. Garvey***, *Donald C. Glaser*

(131) Honorary Session for Prof. Andrew Zydney I

Monday, Nov 8, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 303

Mahsa Rohani, Co-Chair
Ehsan Espah Borujeni, Co-Chair
Ying Li, Co-Chair

Sponsored by: Membrane-Based Separations

12:30 Paper 131i: Remarks by Andrew Zydney — ***Andrew Zydney***
1:00 Paper 255b: Accelerated Product Development and Commercialization in response to the Covid-19 Pandemic: Challenges and Opportunities — ***Manoj Menon***
1:20 Paper 131e: Mechanisms of Protein and DNA Removal in Depth Filtration— *Ohnmar Khanal, Nripen Singh, Steven Traylor, Xuankuo Xu, Sanchayita Ghose,* ***Abraham Lenhoff***
1:40 Paper 199a: Modeling Flux in Tangential Flow Filtration Using a Reverse Asymmetric Membrane for Chinese Hamster Ovary Cell Clarification — ***Ranil Wickramasinghe***, *Da Zhang, Daniel Strauss, Parag Patel, Xianghong Qian*
2:00 Paper 131a: Filtration of Lipid Nanoparticles: The Importance of Understanding Mechanisms to Improve Performance — ***Christina Carbrello***
2:20 Paper 131c: Presentation for Andrew Zydney Honorary Session— ***Parinaz Emami***, *Nuno Pinto, Mark Brower*

(132) In Honor of Erik Ydstie and his Distinguished Academic Career (Invited Talks)

Monday, Nov 8, 12:30 PM
Sheraton Back Bay, Back Bay Ballroom C

Ignacio Grossmann, Chair
Lorenz Biegler, Co-Chair

Sponsored by: Applied Mathematics and Numerical Analysis

12:30: Opening Remarks: Ignacio E. Grossmann
12:35 Paper 132a: Erik Ydstie - His Way — ***Michael F. Doherty***
12:55 Paper 132b: Processes and Systems in the Origin of Life: Thermodynamics and Kinetics — ***Martha Grover***
1:15 Paper 132c: Learning What to Learn: Some Data-Driven Twists in Linking System Identification, Manifold Learning, and (possibly) Causality Considerations — ***Ioannis G. Kevrekidis***, *David Sroczynski, Eleni Koronaki, Felix Dietrich, Noah Wichrowski*
1:35 Paper 132d: Dissipativity Learning Control: Statistical and Control Theoretic Foundations — *Wentao Tang,* ***Prodromos Daoutidis***
1:55 Paper 132e: The Knighthood of the Golden Feedback Loop — ***Blake C. Rawlings***
2:15 Paper 132f: Beyond Learning: What We Learned from Erik — ***Manfred Morari***
2:35: Comments by E. Ydstie
2:45: Closing Remarks: Lorenz T. Biegler

(134) In Honor of the 2019 R.H. Wilhelm Award Winner II (Invited Talks)

Monday, Nov 8, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 210

Amrit Jalan, Chair
C Franklin Goldsmith, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

12:30 Paper 134a: Automating the Construction of Predictive Kinetic Models for the Combustion of Halogenated Hydrocarbons, with Rmg — *David Farina Jr., Sai Krishna Sirumalla,* ***Richard H. West***
12:55 Paper 134b: Unraveling Complex Catalytic Chemistries through Automated Mechanism Generation and Reaction Pathway Analysis — ***Linda Broadbelt***
1:20 Paper 134c: Automated Kinetics for Low-Temperature Oxidation Chemistry— *Amanda L. Dewyer, Maria Demireva, Leonid Sheps,* ***Judit Zádor***
1:45 Paper 134e: Moving from Postdictive to Predictive Kinetics in Reaction Engineering — ***William Green***
2:10 Paper 77d: Chemical Reaction Engineering and Industry: A Match Made in Heaven for Creating a Sustainable Society — ***Kevin Van Geem***

(136) Leaders driving EDI through culture change with stakeholders

Monday, Nov 8, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 301

Gayle Gibson, Chair

Sponsored by: Management Division

(137) Lessons Learned from Teaching Chemical Engineering Online II (How We Changed as Instructors)

Monday, Nov 8, 12:30 PM
Sheraton Back Bay, Republic Ballroom B

Alex Bertuccio, Chair
Amanda Simson, Co-Chair
Jonathan Wenzel, Co-Chair

Sponsored by: Undergraduate Education

12:30 Paper 137a: Replacing Exams with Projects: Advantages and Disadvantages As Observed during Hybrid and Remote Learning and Broader Efforts Towards Equitable Assessment — ***Lucas Landherr***
12:48 Paper 137b: Lessons Learned during the COVID-19 Pandemic: A Literature Synthesis — ***Deja Preusser***, *Milo Koretsky*
1:06 Paper 137c: Interventions to Mitigate Loss of Community during COVID-19— ***Christi Patton Luks***
1:24 Paper 137d: Oral Exams in Undergraduate Cheme Thermo Taught Online— ***Gennady Gor***
1:42 Paper 137e: Online Cheating: A Darker Side of Educational Technology— ***Javier Huayta***, *Zachary S. Campbell, Matthew Cooper*
2:00 Paper 137f: Aiche Education Division Virtual Communities of Practice (VCPs): Updates from the 2020-2021 Academic Year — ***Daniel Lepek***, *Matthew Liberatore*

(138) Materials for Quantum Science

Monday, Nov 8, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 209

Su-Fei Shi, Chair
Carissa Eisler, Co-Chair

Sponsored by: Electronics and Photonics

12:30 Paper 138a: Ultrafast Thermal Transport at Photoexcited 2D Van Der Waals Interfaces (invited) — ***Archana Raja***
1:00 Paper 138b: Stability and Molecular Pathways to the Formation of Spin Defects in Silicon Carbide — ***Elizabeth M.Y. Lee***, *Alvin Yu, Juan J. de Pablo, Guilia Galli*
1:18 Paper 138c: Engineering Spin Dephasing in Metal-Halide Perovskite Nanomaterials for Quantum Information and Spintronics — ***Matthew Crane***, *Laura Jacoby, Theodore Cohen, Daniel Gamelin*
1:36 Paper 138d: Defect Engineering in Hexagonal Boron Nitride Towards Practical Quantum Applications — ***Sylvia Xin Li***, *Michael S. Strano*
1:54 Paper 138e: Orientation Controlled Large Area Epitaxial PbI_2 Thin Films with Tunable Optical Properties — ***Debjit Ghoshal***, *Hanzhi Shang, Tianmeng Wang, Damien West, Nikhil Koratkar, Shengbai Zhang, Su-Fei Shi, Max Lagally*
2:12 Paper 138f: Elucidating the Origin of Intra-Band Optical Transitions in Ag_2se Colloidal Quantum Dots and Their Potential Utilization for Infrared Detectors — ***Ayaskanta Sahu***

(139) Metabolic Platform Development- Non-Conventional Species and Systems

Monday, Nov 8, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 111

Ryan Summers, Chair
Arul Mozhy Varman, Co-Chair

Sponsored by: Bioengineering

12:30 Paper 139a: Synthetic Pathways for Production of 3-Hydroxypropionic Acid and Citramalic Acid in the Non-Model Yeast Issatchenkia Orientalis— ***Patrick Suthers***, *Zia Fatma, Teresa Martin, Zong-Yen Wu, Ye-Gi Lee, Yasuo Yoshikuni, Huimin Zhao, Costas D. Maranas*
12:51 Paper 139b: Metabolic Engineering of *Issatchenkia Orientalis* for Succinic Acid Production — ***Vinh Tran***, *Yihui Shen, Joshua D. Rabinowitz, Huimin Zhao*
1:12 Paper 139c: Consolidated Bioprocessing of Lignocellulosic Biomass Components Via Synergistic Bacterial Co-Culture Consortia — ***Apurv Mhatre***, *Bethany Kalsheur, Thiagarajan Soundappan, Arul Mozhy Varman*
1:33 Paper 139d: Establishing *Eubacterium Limosum* As a Model Methylotrophic Acetogen — *Kathryn Hoyt, Patrick A Sanford,* ***Benjamin Woolston***
1:54 Paper 139e: Model-Guided Design Strategies for Bioplastic Overproduction in Rhodopseudomonas Palustris — ***Adil Alsiyabi***, *Brandi Brown, Rajib Saha*
2:15 Paper 139f: Developing a Novel Microbial Host and Synthetic Biology Tools for Valorizing Waste Polyethylene Terephthalate and Lignin-Derived Compounds — *Jinjin Diao, Yifeng Hu, Drew DeLorenzo, Rhiannon Carr,* ***Tae Seok Moon***
2:36 Paper 139g: Improving *Cupriavidus Necator* As Host for Conversion of Formate to Fuels and Chemicals — ***Christopher Johnson***

(140) Nanomaterials for Energy Storage and Conversion 1

Monday, Nov 8, 12:30 PM
Marriott Copley Place, Simmons

Seung Soon Jang, Chair
Ling Fei, Co-Chair
Tae-Sik Oh, Co-Chair

Sponsored by: Nanomaterials for Energy Applications

12:30 Paper 140a: Development of Ion-Conducting Polymers for Hydrogen Electrochemical Energy Conversion Technologies — ***Chulsung Bae***
12:55 Paper 140b: Coupling Potential Dependency and Spin Effects in Graphene-Based Single Atom Catalysts for Oxygen Evolution and Reduction Reactions — ***Md Delowar Hossain***, *Frank Abild-Pedersen, Michal Bajdich*
1:10 Paper 140c: MOF-Derived $PtCo/Co_3O_4$ nanocomposites in Carbonaceous Matrices As High-Performance ORR Electrocatalysts Synthesized *Via* laser Ablation Techniques — ***Dibyendu Mukherjee***, *Erick L. Ribeiro, Bamin Khomami*
1:25 Paper 140d: Strong *sp-D* Orbital Hybridization Driven Pt-Graphene Hybrid Catalysts for Direct CO_2 Hydrogenation to Formic Acid — ***Jinwon Cho***, *Ji Il Choi, Seung Soon Jang*
1:50 Paper 140e: Computational Design of Active Hybrid Interface Energy Materials from Scratch and Data Science — *Hoje Chun, Sung Jun Hong,* ***Byungchan Han***
2:15 Paper 114d: Controllable Synthesis of Hybrid Nanocomposite Structures *Via* Laser Ablation Technique for Electrochemical Energy Storage and Conversion Devices — ***Mahshid Mokhtarnejad***, *Erick L. Ribeiro, Dibyendu Mukherjee, Bamin Khomami*
2:30 Paper 140h: Enhancing the Performance of Mxene Supercapacitor in Ionic Liquid By Expanding Interlayer Spacing — ***Wei Zhao***, *Ray Matsumoto, Kun Liang, Michael Naguib, Peter Cummings*

(141) Nanostructured Materials for Pharmaceutical Applications

Monday, Nov 8, 12:30 PM
Sheraton Back Bay, Hampton

Timothy M. Brenza, Chair

Sponsored by: Nanoparticles

12:30: Introductory Remarks
12:45: Break
1:00 Paper 141d: Model-Aided Design and Translation of Glucose-Responsive Insulins: From Simple to Complex Mechanisms — ***Jing Fan Yang***, *Naveed Bakh, Xun Gong, Michael S. Strano*
1:15: Break
1:45 Paper 141g: Programmable Biohybrid Nanocarriers for the Sustained Release of Cancer Therapeutics — ***Robert Mosley***, *Jacek Wower, Mark E. Byrne*
2:00 Paper 141h: Self-Organization of Iron Sulfide Nanoparticles into Multi-Compartment Supraparticles — ***Emine Sumeyra Turali-Emre***

(142) New Frontiers of Molecular Thermodynamics (Invited Talks)

Monday, Nov 8, 12:30 PM
Marriott Copley Place, Salon C/D

Sapna Sarupria, Co-Chair
Shikha Nangia, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

12:30 Paper 142a: Single Particle Measurements of Viral Surface Chemistry for Separations and Stability — ***Caryn Heldt***
1:03 Paper 142b: Computer Simulation of Self-Assembly By Multipolar Colloidal Particles and Their Mixtures — ***Carol Hall***
1:36: Break
1:46 Paper 142c: Thermodynamics and Molecular Engineering of Complex Coacervates — ***Sarah L. Perry***
2:19 Paper 142d: Using Simulation to Explore the Effect of Cholesterol on Skin Lipid Self-Assembly — ***Clare McCabe***

(143) NSF Workshop I: Highlights from CBET

Monday, Nov 15, 8:00 AM
Virtual, Education Division (04)

Ram Gupta, Chair
Carole Read, Co-Chair

Sponsored by: Career Guidance Committee Liaison

8:00 Paper 143a: Overview of NSF Chemical, Bioengineering, Environmental, and Transport Systems Division (CBET) — ***Tim Patten***
8:25 Paper 143b: Chemical Process Systems Cluster Overview — ***Ray Adomaitis***
8:45 Paper 143c: Transport Phenomena Cluster Overview — ***Shahab Shojaei-Zadeh***
9:05 Paper 143d: Engineering Biology and Health Cluster Overview — ***Steven Zehnder***
9:25 Paper 143e: Environmental Engineering and Sustainability Cluster Overview — ***Mamadou Diallo***
9:45 Paper 143f: Interactive Question and Answer Session with NSF Program Directors — ***Tim Patten***, *Robert McCabe, Christina Payne, Shahab Shojaei-Zadeh, Steven Zehnder, Mamadou Diallo, Carole Read*

(144) Particulate Systems Dynamics and Modeling: In-person

Monday, Nov 8, 12:30 PM
Sheraton Back Bay, Gardner

Maria. S Tomassone, Chair
Yu Liu, Co-Chair

Sponsored by: Solids Flow, Handling and Processing

12:30 Paper 144e: Understanding Die Compaction of Hollow Spheres Using the Multi-Particle Finite Element Method (MPFEM) — ***Ahmet Demirtas***, *Gerard Klinzing*
12:45 Paper 144i: Access: Autonomous Characterisation and Calibration Using Evolutionary Simulation Software — ***Andrei-Leonard Nicusan***
1:00 Paper 144j: Machine Learning-Based View Factor Modelling in Polydisperse Particle Beds Including Walls — ***Josef Tausendschön***, *Stefan Radl, Gero Stöckl*
1:15 Paper 208c: Transition between Shear-Induced Segregation and Free-Sifting of Fines — ***Song Gao***, *Julio M. Ottino, Paul B. Umbanhowar, Richard Lueptow*
1:30 Paper 208a: Designing Non-Segregating Granular Mixtures for Free Surface Flows — *Yifei Duan, Paul B. Umbanhowar, Julio M. Ottino,* ***Richard Lueptow***
1:45: Break
2:00: Break

(145) Plasma catalysis

Monday, Nov 8, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 306

Ryan Hartman, Chair
Maria Carreon, Co-Chair

Sponsored by: Material Interfaces as Energy Solutions

12:30 Paper 145a: Opening Remarks By the Chair/Co-Chair — ***Ryan Hartman***, *Maria Carreon*
12:33: Break
12:54 Paper 145c: DFT-Informed Energetics of Plasma-Enabled Reactions Pathways and Microkinetic Modeling for Ammonia Synthesis on Transition and Low-Melting Point Metals — *Tsung Wei Liu, Maria Carreon,* ***Diego Gomez Gualdron***
1:15 Paper 145d: Plasma-Assisted Catalytic Approaches for the Production of Chemicals — *Patrick Barboun, Craig Waitt, William Schneider,* ***Jason Hicks***
1:36 Paper 145e: Models and Observations of Plasma-Catalytic Nitrogen Oxidation — *Hanyu Ma, Rakesh K. Sharma, Stefan Welzel, Mauritius C.M. van de Sanden, Mihalis N. Tsampas,* ***William Schneider***
1:57 Paper 145f: Methane-Products Process Intensification through a Nanosecond Plasma Discharge — ***Shayan Niknezhad***, *Efstratios N. Pistikopoulos*
2:18 Paper 145g: Plasma-Assisted Upgrading of Methane: Mechanistic Insights from in-Situ PM-IRAS and OES Spectroscopy — ***Garam Lee***, *Ibukunoluwa Akintola, David Go, Casey O'Brien*

2:39 Paper 145h: Computational Evaluation of Plasmonic Photocatalysis in Au and Ag Nanoparticles — ***Connor Herring***, *Matthew Montemore*

(146) Plenary Session: Crystallization and Evaporation - Area 2B (Invited Talks)

Monday, Nov 8, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 304

Thomas Vetter, Chair
Christopher Burcham, Co-Chair

Sponsored by: Crystallization and Evaporation

12:30: Welcoming Remarks
12:34 Paper 146a: 2020 Honoree Talk: Industrial Crystallization – the Intersection of Solid State Chemistry and Process Engineering — ***Daniel Green***
1:14 Paper 146b: 2021 Honoree Talk: Computational Methods for Crystal Nucleation and Growth: Current Status and Future Directions — ***Baron Peters***
1:54: Presentation of the Graduate Student Researcher Award
1:57 Paper 146c: Modelling Diffusive Mixing in Antisolvent Crystallisation— ***Russell Miller***, *Jan Sefcik, Leo Lue*
2:18 Paper 146d: Development of an Immersion Mill Integrated Crystallization Process Model As Digital Twin for in-Silico Process Optimization — ***Ayse Eren***, *Botond Szilagyi, Justin Quon, Charles D. Papageorgiou, Zoltan Nagy*
2:39 Paper 146e: Secondary Nucleation Rates: Comparison of Mechanisms and Models — ***Luca Bosetti***, *Ramona Achermann, Byeongho Ahn, Marco Mazzotti*

(147) Plenary - In Honor of Professor Paul Steen (Invited Talks)

Monday, Nov 8, 12:30 PM
Sheraton Back Bay, Constitution A

Roseanna Zia, Chair
William Hartt IV, Co-Chair

Sponsored by: Fluid Mechanics

12:30 Paper 147a: Physicochemical Hydrodynamics of Droplets in Inkjet Printing — ***Detlef Lohse***
12:55 Paper 147b: Data-Driven Modeling and Analysis of Complex Flows— ***Michael Graham***
1:20 Paper 147c: My Research Resonance with Professor Paul H. Steen: Dancing Droplets in Outerspace — ***Susan Daniel***
1:45 Paper 147d: Surface Waves on Soft Gels in a Vibrated Cylindrical Container — ***Joshua Bostwick***
2:10 Paper 147e: Statistical Mechanics of the Triple Contact Line — ***Michel Louge***
2:35 Paper 147f: Chasing Flow Instabilities with Paul Steen — ***Steven Weinstein***

(148) Practical Application of Process Data Analytics and Machine Learning (Invited Talks)

Thursday, Nov 18, 8:00 AM
Virtual, Bridging the Skills Gap in Chemical Engineering (T4)

Leo Chiang, Chair
Selen Cremaschi, Co-Chair

Sponsored by: Bridging the Skills Gap in Chemical Engineering

8:00 Paper 148a: Deployment of Machine Learning Models in Pharmaceutical Development — ***Jose Tabora***, *Patrick Sipple*
8:35 Paper 148b: Unsupervised Learning from Sets of Data Using Contrastive Latent Variable Models — ***Kristen Severson***
9:10 Paper 148c: Energy Dispersive X-Ray Hyperspectral Image Analysis and Chemometrics for Catalyst Characterization — ***Jose Maria Gonzalez Martinez***, *Jose Manuel Prats Montalban, R. Haswell, Alberto Ferrer*
9:45 Paper 148d: Applications of machine learning in production enhancement and field monitoring in Oil & Gas industry — ***Haijing Gao***, ***Shuxing Cheng***

(149) Renewable Polymers and Intermediates Technology

Monday, Nov 8, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 300

Danielle Mai, Chair
Shaibal Roy, Co-Chair

Sponsored by: Process Research and Innovation

12:30 Paper 149a: High-Throughput Measurement of a Machine Learning Model for Polyester Biodegradation — ***Sarah Av-Ron***, *Katharina Fransen, Dylan Walsh, Wontae Joo, Bradley Olsen*
12:50 Paper 149b: Buffering Effects on the Solution Behavior and Hydrolytic Degradation of Poly(β-amino ester)s — *Mara Kuenen, James Mullin,* ***Rachel Letteri***
1:10 Paper 149c: Reducing Moisture Sensitivity of Protein-Based Thermosets through Protein Charge Modification and Melt Polymerization with Hydrophobic Monomers — ***Wui Yarn Daphne Chan***, *Emil Andersen, Sarah Av-Ron, Bradley Olsen*
1:30 Paper 149d: Growing Silk Fibroin in Advanced Materials for Food Security— *Hui Sun,* ***Benedetto Marelli***
1:50 Paper 149e: Engineering Charged Silk Conjugates for Ionically Crosslinked Hydrogels — ***Sanyukta Patil***, *Rachel Martineau, Danielle Heichel, Kelly Burke*
2:10 Paper 149f: Renewable Polymers Via Direct Functionalization of Lignocellulosic Sugars — ***Lorenz Manker***, *Graham Dick, Adrien Demongeot, Maxime Hedou, Christele Rayroud, Irina Sulaeva, Yves Leterrier, Antje Potthast, Veronique Michaud, Harm-Anton Klok, Jeremy Luterbacher*
2:30 Paper 149h: Grazing-Incidence Diffraction Reveals Cellulose Lattice Contraction with Dehydration of Plant Primary Cell Wall — ***Joshua Del Mundo***, *Sintu Rongpipi, Hui Yang, Dan Ye, Sarah N. Kiemle, Stephanie L. Moffitt, Charles L. Troxel, Michael F. Toney, Chenhui Zhu, James D. Kubicki, Daniel J. Cosgrove, Esther W. Gomez, Enrique D. Gomez*

(150) Student Competition in Sensors (Sponsored)

Monday, Nov 8, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 200

Kevin Cash, Chair
Stephanie McCalla, Co-Chair
Qingshan Wei, Co-Chair
Han-Sheng Chuang, Co-Chair

Sponsored by: Sensors

12:30 Paper 150a: Power and Lithography Free Highly Sensitive Digital Protein Detection Platform Using an Inexpensive Track-Etched Polycarbonate (PCTE) Membrane — ***Vivek Yadav***, *Himani Sharma, Liao Chen, Satyajyoti Senapati, Hsueh-Chia Chang*
12:48 Paper 150b: Corona Phase Molecular Recognition of Interleukin 6 (IL-6) Using Near-Infrared Single Walled Carbon Nanotube (SWNT) — ***Xiaojia Jin***, *Michael A. Lee, Xun Gong, Naveed Bakh, Minkyung Park, Song Wang, Daichi Kozawa, Sooyeon Cho, Michael S. Strano*
1:06 Paper 150c: Novel Probe for in-Situ Monitoring of Mitochondrial DNA Methylation Reveals Unsynchronized Nucleus and Mitochondria Epigenome Dynamics — ***Han Zhao***, *Donghan Ma, Junkai Xie, Chongli Yuan*
1:24 Paper 150d: Evaluation of Azure a Redox Dye As DNA Hybridization Indicator Using Electrochemical Methods — ***Tugba Yilmaz***, *Edgar D. Goluch*
1:42 Paper 150e: Detection of the Tuberculosis Volatile Organic Biomarker Methyl Nicotinate in Breath Using Electroactive Solutions (EAS) — ***Shaylee Larson***, *Christina Willis, Swomitra Mohanty*
2:00 Paper 150f: Conformable Resonant Sensors for Contact-Free Sweat Analysis through Clothing and Protective Gear — ***Adam Carr***, *Yash Patel, Charles R. Neff, Sadaf Charkhabi, Nathaniel Kallmyer, Hector Angus, Nigel Reuel*
2:18 Paper 150g: A Low-Cost and Facile Color-Changing Nanofilm for Temperature Monitoring and Recording — ***MD Nayeem Hasan Kashem***, *Wei Li*
2:36 Paper 150h: Low-Cost Paper-Based Sensors for Ultra-Fast Room-Temperature Hydrogen Detection Using Palladium Alloy Nanowires— ***Abhishek Kumar***, *Yaoli Zhao, Thomas Thundat, Mark Swihart*

(151) Sustainable Biorefineries Plenary Session (Invited Talks)

Monday, Nov 8, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 312

Eric Tan, Chair
Hasan Atiyeh, Co-Chair
Aida Amini Rankouhi, Co-Chair

Sponsored by: Sustainable Biorefineries

12:30 Paper 151a: Bio-Project "Derisking" through Development of Systematic Methodologies and Frameworks for Risk Assessment — ***Rachel Emerson***, *Jordan Solomon, Marcin Lewandowski, Shyam Nair, Lorenzo Vega-Montoto, Pralhad Burli*
1:15 Paper 151b: Labkey Server for Collaborative, Multi-Center, Data Integration and Analysis in Biorefinery Development — ***Jim Collett***, *Rachel Emerson, David A. Sievers, Robert Kinoshita, Matthew Macduff, Shaun O'Leary*

(152) Sustainable Materials from Lignocellulosic Resources for Industrial Applications

Thursday, Nov 18, 3:30 PM
Virtual, Forest and Plant Bioproducts Division (17)

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

Sponsored by: Forest and Plant Bioproducts Division

3:30 Paper 152a: Characterization of Novel Soybean Hull-Based Binders for Aqua-Feed Pellets — ***Navid Etebari Alamdari***, *Burak Aksoy, Mediha Aksoy, Benjamin Beck, Zhihua Jiang*
3:50 Paper 152b: Biodegradable Plastic Blends from Polyhydroxyalkanoate and Cellulose Ester for Sustainable Packaging — ***Akhilesh Pal***, *Kjeld Meereboer, Manjusri Misra, Amar K. Mohanty*
4:10 Paper 152c: Synthesis of Biobased Phenol-Formaldehyde Wood Adhesives from Biorefinery Derived Lignocellulosic Biomass — ***Archana Bansode***, *Maria Auad*
4:30 Paper 152f: Waste wheat starch-based home compostable plastics for packaging applications — ***Jenna Scharnowski***, *Amar K. Mohanty, Arturo Rodriguez-Uribe, Akhilesh Pal, Tao Wang, Manjusri Misra*
4:50 Paper 152e: A Process to Utilize Rice Straw for High-Value Acoustics Applications — ***Ashutosh Negi***, *Kiran Kumar Adepu, Ejaz Ahmad, M. Ali Haider, S. Fatima*

(153) Technologies for Understanding Microbial Interactions

Monday, Nov 8, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 310

Sujit Datta, Co-Chair
James Wilking, Co-Chair

Sponsored by: Microbes at Biomedical Interfaces

12:30 Paper 153a: High-Throughput and Continuous Chaotic Bioprinting of Spatially-Controlled Bacterial Microcosms — ***Carlos Fernando Ceballos-González***, *Edna Johana Bolívar-Monsalve, Diego Alonso Quevedo-Moreno, Li Lu Lam-Aguilar, Karen Ixchel Borrayo-Montaño, Juan Felipe Yee-de León, Y. Shrike Zhang, Mario Moisés Álvarez, Grissel Trujillo de Santiago*

1:00 Paper 153b: Targeted Disruption of Dual Species Interfacial Films of *P. Aeruginosa* and *S. Aureus* — ***Sricharani Balmuri***, *John Simonelli, Tagbo H. R. Niepa, PhD*
1:30 Paper 153c: In Situ Mapping of the Mechanical Properties of Sulfate Reducing Bacteria By Microrheology — *Maryam Amouamouha, Jawahar R. Kalimuthu, Shankarachary Ragi,* ***Travis W. Walker***
2:00 Paper 153d: Polymer Surface Dissection for Characterization of Early Colonizing Microbes on Membrane Interfaces — ***Ryan Hansen***, *Mohammadali Masigol, Prathap Parameswaran, Esther Radaha*
2:30 Paper 153e: Titanium Wires Modified By Peptoid-Loaded Microgels Resist *S. Aureus* Colonization — ***Wenhan Zhao***, *Xixi Xiao, Jennifer S. Lin, Annelise E. Barron, Lauren De Stefano, Jordan Katz, Matthew Libera*

(154) Transport Processes in Chemical Reactors

Monday, Nov 8, 12:30 PM
Sheraton Back Bay, Constitution B

Ravindra Aglave, Chair

Sponsored by: Transport and Energy Processes

12:30 Paper 216b: Design and Evaluation of Nonthermal Plasma Reactors for Hydrogen Production from Polyethylene — ***Benard Tabu***, *Kevin Akers, Peng Yu, Mammadbaghir Baghirzade, Eric Brack, Christopher Drew, J. Hunter Mack, Hsi-Wu Wong, Juan Trelles*

(155) Two-Dimensional Materials and Thin Films

Monday, Nov 8, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 105

Dongxia Liu, Chair
Mark Snyder, Co-Chair
Kumar Varoon Agrawal, Co-Chair
Seokjhin Kim, Co-Chair

Sponsored by: Inorganic Materials

12:30 Paper 155a: Bottom-up Synthesis of Films Hosting Atom-Thick Molecular-Sieving Apertures — *Kumar Varoon Agrawal,* ***Luis Francisco Villalobos***
1:00 Paper 155b: Xenon Trapping in Silica Nanocages Supported on Ru(0001)— *Yixin Xu,* ***Matheus Dorneles de Mello***, *Chen Zhou, Burcu Karagoz, Ashley Head, Zubin Darbari, Iradwikanari Waluyo, Adrian Hunt, Dario Stacchiola, Sergio Manzi, Alejandro Boscoboinik, Victor Pereyra, Jorge Boscoboinik*
1:20 Paper 155c: Tuning 3D Assembly of Ti_3C_2 Mxene Nanosheets through Mxene/Polyelectrolyte Complexation — ***Farivash Gholamirad***, *Nader Taheri-Qazvini*
1:40 Paper 155d: Tuning d-Spacing of Graphene-Oxide Via Covalent Crosslinking with Triaminotriptycene for Improved Water Stability and Molecular Sieving — ***Moonjoo Lee***, *Hyunhee Lee, Shaofei Wang, Pan Wang, Intak Jeon, Timothy Swager, Zachary Smith*
2:00: Break
2:20 Paper 155f: Control Release of Edge and Basal-Plane-Specific Kinetics of Planar, 1D Wrinkled, and 2D Crumpled Nanochannels of Graphene Oxide Films Intercalated — *Muchun Liu,* ***Deisy Cristina Carvalho Fernandes***, *Zachary Saleeba, Robert Hurt*
2:40 Paper 155g: Visualizing Oxidation Mechanisms in Few-Layered Black Phosphorus Via in Situ Transmission Electron Microscopy — ***Piran Kidambi***

(156) Wilson Award Presentation (Invited Talks)

Thursday, Nov 18, 12:30 PM
Virtual, Nuclear Engineering Division (14)

Philip Schonewill, Chair
James Laurinat, Co-Chair

Sponsored by: Nuclear Engineering Division

12:30 Paper : Reprocessing of Highly Enriched Aluminum-clad Fuels in the Savannah River Site H-Canyon Facility: Past, Present, and Future — ***Tracy S. Rudisill***
1:30: Q&A

(157) MAC 30th Anniversary Session

Monday, Nov 8, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 209

Sponsored by: Minority Affairs Committee (MAC)

(158) The Langer Prize for Innovation and Entrepreneurial Excellence Award Presentation and Lecture

Monday, Nov 8, 1:45 PM
John B. Hynes Veterans Memorial Convention Center, Ballroom B

Sponsored by: Awards Committee

1:45: Session Welcome & Introduction – Pablo Debenedetti
2:00: Remarks from Bob Langer
2:10: 2020 and 2021 Prize Presentation
2:20: Remarks from María Eugenia Inda, 2020 Langer Prize Fellow
2:25: Remarks from Aditya Kunjapur, 2021 Langer Prize Fellow
2:50: Closing Remarks - Terry McGuire & Amy Schulman
2:55: Networking & Light Refreshments

(159) General Poster Session

Monday, Nov 8, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, Exhibit Hall C/D

Sponsored by: Poster Sessions

Poster 711c: Analysis of Fluid Motion and Performance of Simulated Moving Bed with Different Design of Flow Distributor — ***Youngjin Kim***, *Jaewon Lee, Myungjun Kim, Il Moon*
Poster 685d: Field Wide Optimisation for Improved Hydrocarbon Recovery— ***Shakeel Ramjanee***
Poster 699d: Regeneration of Methane Dehydroaromatization Using Periodic and Pulse Feeding of CO_2 and H_2 — ***Nagat Elrefaei***, *Mamoun Al-Rawashdeh*
Poster 159a: Amphiphilic Block Copolymers as Modulators of Interfacial Tension for Biosensing — ***Tyler Durkin***, *Suchol Savagatrup*
Poster 159b: Reconfigurable Complex Emulsions for Rapid, Real-Time, and Multiplexed Sensing Array — ***Baishali Barua***, *Suchol Savagatrup*
Poster 159c: Development of catalysts for removal of sulfur compounds from natural gas — ***Percival Soni Castro***, *Rafael Hernandez, William Holmes, Mark Zappi, August Gallo, Daniel Gang*
Poster 159g: Effect Study of Operating Conditions and Optimization of Gas Holdup in a Bubble Column Reactor — ***Ghanim M. Alwan Sr.***, *Muthanna H. Aldahhan*
Poster 159k: Modification of 13X Zeolite Via Molecular Layer Deposition for Post Combustion CO2 Capture — ***Richard Ciora***, *Miao Yu, Shoujie Ren*
Poster 159l: Mixture Solubility Parameters from Experimental Data and Perturbed-Chain Statistical Associating Fluid Theory — ***Joseph R. Vella***, *Bennett Marshall*
Poster 159m: Graphene Oxide-Carbon Nanotube Hybrid Membranes for Organic Solvent Separation Using Membrane Distillation — ***Oindrila Gupta***
Poster 159n: Computational Fluid Dynamics Simulation Study to Resolve Mixing Challenges of Non-Newtonian Fluids in Pharmaceutical Industry— ***Nikhil Srivastava***, *Saurav S. Rath, SVB Janardhan Garikipati, Birendra K. David*
Poster 159r: Design and Optimisation of Highly Efficient Catalysts for Gas Phase CO_2 Recycling — ***Laura Pastor-Perez***, *Jesus Gandara Loe, Tomás Ramirez-Reina, José Antonio Odriozola*
Poster 159t: Discerning in Vitro Pharmacodynamics from Optical Density Measurements: A Model-Based Approach — ***Iordanis Kesisoglou***, *Vincent H. Tam, Andrew P. Tomaras, Michael Nikolaou*
Poster 159u: Monitoring Carbon Dioxide for Carbon Capture, Utilization, and Storage (*CCUS*) Applications — ***Richa Sharma***, *T. S. Ramakrishnan, Quincy K. Elias*
Poster 159v: Experimental and Theoretical Screening of Transition Metal Catalysts for Electrochemical Oxidation of Nitrogen to Nitrates — ***Nishithan Balaji Chidambara Kani***, *Meenesh Singh*
Poster 159w: Synthesis of Sludge Based Mesoporous Carbon for the Degradation of Rhodamine B Using Sodium Percarbonate Activation: Electron Transfer Mechanism — ***Muhammad Danish***, *Usman Farooq, Shuguang Lu*
Poster 159x: Lipase Immobilization on Mesoporous Carbon and Evaluation As Catalysts in the Hydrolysis of Waste Oleochemical Streams. — ***Alexander Baena***, ***Alvaro Orjuela***
Poster 159z: Engineering Oxygen Vacancies at Metal-Oxide Interface By Depositing Ultra-Thin ZrO_2 Overcoating on Ni/Al_2O_3 for Dry Reforming of Methane — ***Baitang Jin***, *Shiguang Li, Yuzi Liu, Xinhua Liang*
Poster 159ae: Process Engineering Design of Tobacco Wastes Incinerator with Utilization of Heat Energy from Combustion Gases — *Asmaa Elmansy, Nabil Abdelmonem, Ahmed Shaaban,* ***Amr Abdelghany***
Poster 159af: Field Wide Optimization for Improved Upstream Hydrocarbon Recovery — ***Shakeel Ramjanee***
Poster 159ag: Removal of Cadmium (II) from Aqueous Solution By Adsorption on an Hydrochar Prepared from Water Hyacinth — ***Carolina Vazquez-Mendoza***, *Roberto Leyva-Ramos, Nahum A. Medellin-Castillo, Araceli Juarez-Martinez*
Poster 159al: Time-Lapse –Reservoir Simulation Calibration Using Vsp Seismic Data from Farnsworth Unit, Texas. — ***Samuel Acheampong***, *Robert Will, William Ampomah, Hassan Khaniani*
Poster 159am: Plasma Synthesized Gallium Nitride Nanoparticles for Wavelength-Tunable Photoluminescence — ***Dillon Moher***, *Elijah Thimsen*
Poster 159ar: How Low Can It Go?: Survivability of Aerobic Activated Sludge Fed Dilute-Strength Wastes for Space Applications — ***Nicholas Marcil***, *Mark Zappi, Dhan Lord Fortela, Emmanuel Revellame, Daniel Gang, Wayne Sharp, William Holmes, Rafael Hernandez*
Poster 159at: Probing the Influence of Bubble Generation on the Rate of Gas Evolution in Super-Saturated Silicone Oils — ***Anirban Ghosh***, *Michael Miranda, Clint Aichele*
Poster 159av: Water Desalination through the Selective CVD Graphene-Based Membrane — ***Mansour Saberi***, *Stephen Creager*
Poster 159ay: Atomically Thin Graphene Membranes with Nanoscale Pores for Dialysis Based Separations — ***Piran Kidambi***
Poster 159az: Modeling the Onset of Symptoms of COVID-19: Effects of Sars-Cov-2 Variant and Patient Comorbidities — ***Joseph Larsen***, *Margaret R. Martin, John D. Martin, James B. Hicks, Peter Kuhn*
Poster 159ba: Anti-biofilm Activity of Chiral Graphene Quantum Dots and Their Effects on Functional Bacterial Amyloid Proteins — ***Misché Hubbard***, *Christopher Altheim, J. Scott Van Epps, Nicholas Kotov*
Poster 159bb: A Continuous-Time Linear Programming Formulation for the Resource-Constrained Project Scheduling Problem with Production and Consumption of Resources — ***Norbert Trautmann***, *Mario Gnägi*
Poster 159bd: Highly stable Pt-Co bimetallic catalysts prepared by atomic layer deposition for cinnamaldehyde selective hydrogenation — ***Kaiying WANG***, *Xiaoqing He, Jee-Ching Wang, Xinhua Liang*

(160) Poster Session: Bioengineering

Monday, Nov 8, 3:30 PM

John B. Hynes Veterans Memorial Convention Center, Exhibit Hall C/D

Andrew Jones, Chair
John Blazeck, Co-Chair
Jason Boock, Co-Chair
Nicholas Sandoval, Co-Chair

Sponsored by: Bioengineering

Poster 536f: The Effect of Fat Concentration on the Microbial Dynamics and Bacterial Biofilm Development on a Novel Viscoelastic Triphasic Food Model— ***Lisa Purk***, *Melina Kitsiou, Katherine Costello, Jorge Gutierrez-Merino,* ***Eirini Velliou***

Poster 160b: Impact of Ammonia Stress and Cell Line Age on Glycosylation of CHO-Derived VRC01 Monoclonal Antibody — *Claire McGraw, Benjamin Synoground,, Kathryn Elliott, Jada Roth, Sarah W. Harcum,* ***Nicholas Sandoval***

Poster 160c: Studying Phenotype Differences of Prostate Cancer Cells Using Electrical Impedance Spectroscopy — ***Lexi Crowell***, *Tunglin Tsai, Brian Aufderheide, Juan Sebastian Yakisich, Tayloria Adams*

Poster 160d: Acute Exposure to E-Cigarette Vapor Promotes Neutrophil/Platelet Aggregation in Pulmonary Microvasculature — ***Hunter Snoderly***, *Hassan Alkhadrawi, Margaret Bennewitz*

Poster 160e: Electrochemically Regulated Polyelectrolyte Complex for Smart Wound Dressings — ***Asma Allababdeh***, ***Byung-Wook Park***

Poster 160g: Monitoring Cancer Progression during Treatment Via Size-Based Sorting of Exosomes — ***Olivia Buraks***, *Qingxuan Li, Ming Su*

Poster 160h: Surrogate-Based Feasibility Analysis for the Identification of Design Space of Multicolumn Counter-Current Continuous Protein a Chromatography — ***Chaoying Ding***, *Marianthi Ierapetritou*

Poster 160k: Engineering "Designer" Biologics in Plant Cells for Oral Treatment of Inflammatory Bowel Disease — *Wenzheng Guo, Carmela UnnoldCofre,* ***Jianfeng Xu***

Poster 160n: Computational RNA Design in the Ribosomal Active Site— ***Camila Kofman***, *Andrew Watkins, Alex Wooldredge, Rhiju Das, Michael Jewett*

Poster 160o: Bench-Scale Production of Glutaraldehyde Polymerized Bovine Hemoglobin with Tunable Biophysical Properties As a Red Blood Cell Substitute— ***Xiangming Gu***, *Crystal Bolden-Rush, Andre Palmer*

Poster 160p: Surface Camouflaged *Lumbricus Terrestris* mega-Hemoglobin for Diverse Oxygen Therapeutic Applications — ***Chintan Savla***, *Andre Palmer*

Poster 160r: Hydrolyzed Collagen Hydrogels Development for Cosmetic Applications — ***Maoqi Feng***, *Songqing Lu*

Poster 160s: Optimized Tip-Sonication Temperature and Mixing Using Finite Element Modeling for High-Yield Bacterial Cell-Free Extract — ***Md Sakib Ferdous***, *Jared Dopp, Nigel Reuel*

Poster 160u: Development of a high-density perfusion bioreactor production unit using scale-down models and marine bacterium Rhodovulum sulfidophilum for the production of therapeutic oligonucleotides — ***João Medeiros Garcia Alcântara***, *Michele Chen, Fani Sousa, Davide Moscatelli, Mattia Sponchioni, Massimo Morbidelli*

Poster 160v: Development of a Transcriptional Biosensor for Interrogating the Role of Hydrogen Sulfide in IBD Onset — ***Matthew T. Fernez***, *Benjamin Woolston*

Poster 160w: Optimizing Needle-Free Jet Injections for Intradermal Delivery— ***Pankaj Rohilla***, *Jeremy Marston*

Poster 160x: Amplification-Free Nucleic Acid Detection at Room Temperature Using CRISPR Chain Reaction — ***Santosh Rananaware***, *Emma Vesco, Grace Shoemaker, Nicolas Macaluso, Swapnil Anekar, Marco Downing, Piyush Jain*

Poster 160z: Interaction Study of Myoglobin and Chlorpyrifos — ***Shalini Shikha***, *Sudip Pattanayek*

Poster 160aa: Reliability and Reproducibility of Amplification in Rapid PCR-Based Nucleic Acid Testing — ***MInGin Kim***, *Victor M. Ugaz*

Poster 160ab: Development of Stable Targeted Nano-, Encapsulated Manganese Oxide (NEMO) Particles for Early Breast Cancer Diagnosis By MRI— ***Celia Martinez de la Torre***, *Kasey Freshwater, Margaret Bennewitz*

Poster 160ad: Toxicokinetic Interactions of Industrial Chemical Mixtures As Internal Exposure Modifiers — *Dimosthenis Sarigiannis, Ioannis Petridis, Venetia Kokaraki, Alberto Gotti,* ***Spyros Karakitsios***

Poster 160af: Development of a Luciferase Reporter Assay for Real-Time Monitoring of *Streptococcus Pyogenes* Cysteine Protease S*peb* Transcription— ***Lena Young***, *Lucas Peck, Juan Nevarez, Elena Holley, Michael Watson*

Poster 160ag: *In Vivo* Biosynthesis of Dimethyltryptamine (DMT) in *E. coli*— ***Lucas Friedberg***, *Andrew Jones, Abhishek Sen*

Poster 160ah: Metabolic Engineering Techniques to Enable and Increase *De Novo* Production of Psilocybin in *E. coli* — ***Nicholas Kaplan***, *Jack Verderber, Andrew Jones*

Poster 160ai: Analyzing *in-Vivo* Enzyme Activity to Optimize Recombinant Microbial Fermentation — ***Abhishek Sen***, *Andrew Jones*

Poster 160aj: Production of Non-Natural, Bioactive, and Potentially Therapeutic Tryptamines Using the Psilocybin Biosynthesis Pathway in an *E. coli* Host— ***William Gibbons Jr.***, *Andrew Jones*

Poster 160ak: Transposon Mediated and Cas9 Assisted Integration and Promoter Optimization of Psilocybin Biosynthetic Pathway — ***Philip O'Dell***, *Ben Powell, Andrew Jones*

Poster 160al: Medium Throughput Combinatorial Gene Knockout Strategy to Improve Polyketide Production — ***Hannah Yocum***, ***Anhuy Pham***

Poster 160am: Transcriptome-Guided Mining and Functional Characterization of paclitaxel Transporters in *Taxus* Plant Cell Culture — ***Cassandra Brzycki***, *Sangram Lenka, Lexi Crowell, Huilin Yang, Mariana Harley, Eric Young, Susan Roberts*

Poster 160an: Bioconversion of Formic Acid in Escherichia coli Using a 2-Hydroxyacyl-CoA Lyase (HACL)-Based Pathway — ***Fayin Zhu***, *Seung Hwan Lee, Alexander Chou, James M. Clomburg, Ramon Gonzalez*

Poster 160ao: Nucleotide Sugar Production By Engineered Yeast — ***Shuyuan Zhang***, ***Ryan Summers***

Poster 160ap: Investigation of Co-Substrate Utilization By *E. Limosum* for Biofuel Applications — ***Kathryn Hoyt***, *Benjamin Woolston*

Poster 160ar: Directed Genomic Engineering of Pichia Pastoris Cell Wall to Enhance Protein Secretion — ***Hayley Ford***, *Neil Dalvie, Carmen Elenberger, Timothy Lorgeree, J. Christopher Love*

Poster 160as: Development and Optimization of a Flexible Methanol-Free Protein Expression System for *Pichia Pastoris* — ***Andrew Biedermann***, *Neil Dalvie, Isabella R. Gengaro, Timothy Lorgeree, Kerry Routenberg Love, J. Christopher Love*

Poster 160at: Quinolactacin Biosynthesis Involves Nrpss Catalyzed Dieckmann Condensation to Form the Quinolone-Γ-Lactam Hybrid — ***Fanglong Zhao***

Poster 160av: Computational Design for the Lengthening and Widening of Beta Roll-Forming Peptides for Emerging Biotechnology Applications — ***Virginia Jiang***, ***Matthew Lucia***, ***Devin Golla***, *Farid Khoury, Scott Banta*

Poster 160aw: Expanding Promoter Options to Engineer an Environmental-Isolate of *Bacillus Megaterium* — ***Elaine Reece***, *Adam J. E. Freedman, Yoseb Song, Michael T. Timko, Janelle Thompson, Kristala Prather, Jason Boock*

Poster 160ax: Investigating the Role of pBBR1's Mobilization Protein in Plasmid Maintenance in Nonmodel Bacteria — ***Mark Kathol***, *Cheryl Immethun, Rajib Saha, Dianna Long*

Poster 160bc: Machine Assisted Experimentation for Extrusion-Based Bioprinting — ***Shuyu Tian***, *Rory Stevens, Bridget McInnes, Nastassja Lewinski*

Poster 160bd: A Technical Review of Respiratory Infection Mathematical Models in the Context of Sex-Specific Outcomes — ***Tatum McGeary***, *Jason E. Shoemaker*

Poster 160bg: Layered Feedback Control Overcomes Performance Trade-off in Synthetic Biomolecular Networks — ***Chelsea Hu***, *Richard M. Murray*

(161) Poster Session: Engineering Fundamentals in Life Science

Monday, Nov 8, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, Exhibit Hall C/D

Shreyas Rao, Co-Chair
Whitney Stoppel, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

Poster 161a: Bacterial Expression of Moringa Oleifera Seed Proteins for Virus Filtration — ***Brielle Hohne***, *Laxmicharan Samineni, Manish Kumar*

Poster 161b: Analysis of How Mutations Disrupt Hotspot Binding Interactions— ***Sumaiya Islam***, *Robert Pantazes*

Poster 161c: Co-Assembling Oppositely Charges Peptides for Salt Bridge Analysis — ***Handan Acar***

Poster 161d: Colocalization of Enzymes on the Yeast Peroxisome Surface to Improve Polyketide Production — ***Hannah Yocum***

Poster 161f: The Impact of Spacer Length on the Morphology and Internalization of MUC1 Aptamer-Amphiphile Nanoparticles for Targeting and Imaging Triple Negative Breast Cancer Cells — ***Zachary Schneiderman***, *Huihui Kuang, Ahmed Shabana, Gabriella Russo, Jun Guo, Denis Wirtz, Efrosini Kokkoli*

Poster 161g: Corona Charge Combined with Moderate Temperature Increases for the Transfection of T-Cells I*n Vitro* — ***Molly Skinner***, *Mark J. Jaroszeski*

Poster 161i: 3D Cellular Microarray Platform for Human Induced Pluripotent Stem Cell Culture and Toxicology Screening — ***André Lopes Rodrigues***, *Vibha Narayanan, Sneha Gopal, Tiago G. Fernandes, Maria Margarida Diogo, Joaquim M.S. Cabral, Jonathan S. Dordick*

Poster 161n: Evaluating Parameters Associated with the Activation of Immune Response in Phosphatidylserine Targeted Photothermal Therapy of Triple Negative Breast Cancer Tumor Model in Mice — ***Gabriela Faria***, *Clément G. Karch, Alexis Woodward, Adam Aissanou, Patrick McKernan, Roger Harrison*

Poster 161o: In-House v. Commercialized Cores for Nano-, Encapsulated, Manganese Oxide (NEMO) Particles As MRI Contrast Agents — ***Kasey Freshwater***, *Celia Martinez de la Torre, Margaret Bennewitz*

Poster 161p: Modulating the Single-Bacterium Adhesion Behavior Via Regulation of Extracellular Electron Transfer — ***Shuomeng Zhang***, *Lei Wang, Liang Wu, Zhongjian Li, Qinggang He*

Poster 161q: Effects of Sustained Low-Dosage Aspirin Consumption on the Mechanical Properties of Human Blood - a Rheological Study — *Trevor Corrigan,* ***Liam O'Malley***, *Thomas Brown, Dorian Bailey, Hope Moseley, Minseo Yang, William Chang, Thomas Batt, Anthony Amaru, J Okaikoi, Emily Dinallo, Sean Murray, Erin Milner, Kevin O'Donovan, Matthew Armstrong*

Poster 161r: Computational Fluid Dynamics Simulation Study to Resolve Mixing and Scale-up Challenges of Non-Newtonian Fluids in Pharmaceutical Industry— ***Nikhil Srivastava***, *Saurav S. Rath, SVB Janardhan Garikipati, Birendra K. David*

Poster 161s: Dynamic Gene Control through Interallelic Interactions in Drosophila Embryos — ***Hao Deng***, *Bomyi Lim*

Poster 161t: Interplay between Chemotactic Dispersal and Biofilm Formation in Bacterial Communities — ***Jenna Ott***, *Selena Chiu, Daniel B. Amchin, Tapomoy Bhattacharjee, Sujit Datta*

Poster 161u: Directed Evolution of Polymers through Combinatorial Design & Statistical Learning: Applications in Gene Editing — ***Ramya Kumar***

(162) Poster Session: Food and Bioprocess Engineering

Monday, Nov 8, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, Exhibit Hall C/D

Sitanan Thitiprasert, Chair
Nuttha Thongchul, Co-Chair
Teng Bao, Co-Chair

Sponsored by: Food

Poster 162f: Characterization of Cellulose Biopolymer Synthesizing Enzymes Reconstituted *in Vitro* — ***Dharanidaran Jayachandran***, *Shishir Chundawat*

(163) Poster Session: Interfacial Phenomena (Area 1C)

Monday, Nov 8, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, Exhibit Hall C/D

Christopher Wirth, Chair
Marina Tsianou, Co-Chair

Sponsored by: Interfacial Phenomena

Poster 163a: Janus Particles Swimming Along Solid and Liquid Boundaries— ***Baseemah Rucker***, *Ilona Kretzschmar*
Poster 163b: Leveraging Kosmotropic Aggregation of Silk Fibroin to Promote Continuous Nano-Thin Coating Formation — ***Caleb Wigham***, *Tanner D. Fink, Jeongae Kim, R. Helen Zha*
Poster 163d: Synthesis and Deposition of Microscale Capsules — ***Hairou Yu***, *Christopher Wirth*

(164) Poster Session: Materials Engineering & Sciences (08A - Polymers)

Monday, Nov 8, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, Exhibit Hall C/D

Santanu Kundu, Chair
Iman Noshadi, Co-Chair
Jessica Schiffman, Co-Chair
Evan Wujcik, Co-Chair

Sponsored by: Polymers

Poster 31d: Heterogeneous Nucleation in Polyethylene: Experiments and Molecular Simulations — ***Nathan Volchko***, *Gregory Rutledge*
Poster 643i: Phase Inversion Prediction during the Bulk Synthesis of High-Impact Polystyrene: A Fluid-Dynamic Approach — ***Juan Maffi***, *Diana A. Estenoz*
Poster 164ab: Effect of Temperature and Monomer Addition on Rheological Properties of Chiral Cellulose Nanocrystals Suspensions — ***Mohsen Esmaeili***, *Kyle George, Nader Taheri-Qazvini, Monirosadat Sadati*
Poster 164b: Evaluation of Structural and Photonic Properties of Tunicate-Derived Cellulose Nanocrystals — ***Kyle George***, *Mohsen Esmaeili, Monirosadat Sadati*
Poster 164c: Starch-Based Viscosity Modifying Agents of Mortar — ***Andrea González-Córdoba***, *Paulo Cesar Narvaez Rincon, Jairo E. Perilla*
Poster 164r: Development of Energy Efficient, Photocatalytic and Eco-Friendly Roof Tiles — ***Maria Kouroutzi***, *Antonios Stratidakis, Marianthi Kermenidou, Spyros Karakitsios, Denis Sarigiannis*
Poster 164e: Updating Classical Polymer Network Swelling Theory with Loop Defects — ***Haley Beech***, *Nathan Rebello, Bradley Olsen*
Poster 164g: A Novel Self-Consistent Field Theory Formalism for Sequence-Defined Copolymers — ***Oliver Xie***, *Bradley Olsen*
Poster 164h: Aqueous Electrochemistry of Conducting Polymers at Low Temperatures — ***Lekha Papammagari***, *Sanjeev Manohar*
Poster 164l: A Reappraisal of Typical and Novel Fiber Forming Polymeric Materials — *Rajni Bala Talwar*, ***Nikhil Prakash***
Poster 164m: Evaluation of Residual Surfactant in Polymeric Nanoparticles By Tmdsc — ***Guangliang Liu***, *Kathleen McEnnis*
Poster 164n: Effect of Sticker Clustering on Self-Diffusion in Associative Polymer Gels Revealed By Brownian Dynamics Simulation — ***Ameya Rao***, *Jorge Ramirez, Bradley Olsen*
Poster 164s: Plasticization in Thermally Rearranged Polymers: Effect of Free Volume Elements and Chain Dynamics from Molecular Dynamics Simulations— ***Mohammed Al Otmi***, *Janani Sampath*
Poster 164w: Ph- and Salt-Dependent Phase Composition Measurements of Two-Phase Mixtures of Oppositely Charged Polyelectrolytes Using C-NMR— ***Ying Liu***, *Ronald Larson*
Poster 164t: Understanding Processing Effects during Solution Deposition of Polymer Blends — ***Dongjoo Lee***, *Rafael Verduzco*
Poster 164v: Molecular Dynamics Simulation of Nafion Configurations to Improve O2 Transport — ***Nicholas Tiwari***, ***Xiaoxiao Wang***
Poster 164x: Polymerized Bi-Continuous Microemulsions As Ultrafiltration Membranes — ***Muhammad Azeem Ur Rehman Alvi***, *Reza Foudazi*
Poster 164a: Solid-Supported Photoredox Catalysis for Continuous Flow Reactors — ***Sarah Freeburne***, *Kirsten Bell, Christian Pester*
Poster 164z: A Stochastic Chemical Search Grammar for Macromolecules— ***Nathan Rebello***, *Tzyy-Shyang Lin, Bradley Olsen*
Poster 164d: Conjugated Grafted Polymers for Electrochemical Transistors— ***Ashley Masucci***, *Christian Pester, Enrique D. Gomez*
Poster 164aa: Development of a Rubber Recycling Process Based on a Single Component Interfacial Adhesive — *Michelle Calabrese, Wui Yarn Daphne Chan*, ***Sarah Av-Ron***, *Bradley Olsen*
Poster 164ae: Shear-Responsive Adhesion and Detachment of Dendrimer Coatings on Nano- and Micro-Particles — ***Srivatsan Ramesh***, *Ryan Smith, Christopher Gorman, Stefano Menegatti*

(165) Poster Session: Materials Engineering & Sciences (08B - Biomaterials)

Monday, Nov 8, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, Exhibit Hall C/D

Jungwoo Lee, Chair
Evan Wujcik, Co-Chair
Jessica Schiffman, Co-Chair

Sponsored by: Biomaterials

Poster 165c: Defect Engineering of Enzyme-Embedded Metal-Organic Frameworks for Smart Cargo Release — ***Yi Feng***
Poster 165h: Characterization of LL37 Binding to Collagen through Collagen-Binding Domains (CBDs) — ***Ziqi Wei***, *Marsha W. Rolle, Terri A. Camesano*
Poster 165i: Molecular Dynamic Simulation of Self-Assembly and Mechanical Deformation of Silk Fibroin — ***Jeongae Kim***, *Yanming Zhang, Yunfeng Shi, R. Helen Zha*
Poster 165j: Synthesis of Active Fusion Protein Nanosheets — ***Dylan Dautel***
Poster 165k: Mimicking the Nucleus: Stimuli-Responsive Coacervate Formation and Dissolution in a Microcapsule — ***Faraz Burni***, *Srinivasa R. Raghavan*
Poster 165l: Understanding Membrane Permeability of Proteinosomes Self-Assembled from Globular Fusion Proteins — ***Jackson Powers***, *Blair Cole, Seok Hoon Hong, Yeongseon Jang*
Poster 165n: A Molecular Dynamics-Based, Molecular Thermodynamic Model to Pre-Screen Tomorrow's Vaccines — ***Luke Kruse***, *Karl Hammond, Bret Ulery*
Poster 165o: Water-Responsive Actuation of Gram-Negative/-Positive Bacterial Peptidoglycan — ***Haozhen Wang***, *Zhi-Lun Liu, Seungri Kim, Xi Chen*
Poster 165p: Continuous Chaotic Bioprinting of Skeletal Muscle-like Constructs— ***Edna Johana Bolivar-Monsalve***, *Carlos Fernando Ceballos-González, Karen Ixchel Borrayo-Montaño, Diego Alonso Quevedo-Moreno, Juan Felipe Yee-de León, Ali Khademhosseini, Paul Weiss, Mario Moisés Álvarez, Grissel Trujillo de Santiago*
Poster 165r: Erosion Studies of Poly(sebacic acid and lactic acid) Copolymeric Drug Delivery Vehicles — ***Eswar ArunKumar Kalaga***, *Timothy Brenza*
Poster 165s: Effective Coverage Characterization of Surface-Immobilized Elastin-like Peptides (ELP) for Electrochemical Applications in Varying Conditions — ***Zihang Su***, *Chul-Oong Kim, Julie N. Renner*
Poster 165u: Combinatorial Approach to Assess Self-Assembly Dynamics and Structure Properties of Alkyl Chain Modification of Hyaluronic Acid Hydrogels— ***Jordan Chapman***, *Cerasela Zoica Dinu*
Poster 165v: Rheological Properties of Hydrogels for Controlled Drug Delivery— ***Hossein Hosseini***, *Faezeh Aghazadeh Dizaji*
Poster 165z: Abstract: Engineering of Heparin/Collagen Microcarrier Coatings for Human Mesenchymal Stromal Cells Manufacturing — ***Hemanta Timsina***, *Jorge Almodovar*
Poster 165x: Regulation of Stem Cell Spheroid Function in Gelatin Methacryloyl Hydrogel with Different Mechanical Properties for 3D Tissue Engineering — ***Eun Mi Kim***, *Heungsoo Shin, Hyunjoon Kong*
Poster 165y: A Physiologically Relevant 3D in-Vitro Model of Retinal Degenerative Diseases — ***Ronak Ansaripour***, *Joydip Kundu, Shun Zhang, Petr Baranov, Julia Oswald, Roger D. Kamm, Rebecca L. Carrier*
Poster 165w: Biodegradable Nanofiber Bone-Tissue Scaffold As Remotely-Controlled and Self-Powering Electrical Stimulator — ***Ritopa Das***, *Thanh Nguyen*
Poster 165ab: Crosslinking to Enhance the Mechanical Properties of 3D-Plotted Collagen-Based Scaffolds for Bone Tissue Engineering — ***Jackson Conroy***, *Greta Schwartz, Paul F. James, Azizeh-Mitra Yousefi*
Poster 165aa: Degradable Oxidized Alginate Microbeads Promote Cell Viability and Extracellular Matrix Synthesis within Genipin-Crosslinked Fibrin Composite Hydrogel Constructs — ***Chris Panebianco***, *Sanjna Rao, Jennifer Weiser, James Iatridis*

(166) Poster Session: Materials Engineering & Sciences (08D - Inorganic Materials)

Monday, Nov 8, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, Exhibit Hall C/D

Xueyi Zhang, Chair
Satish Nune, Co-Chair
Evan Wujcik, Co-Chair
Jessica Schiffman, Co-Chair

Sponsored by: Inorganic Materials

Poster 166a: Simulation of the Interface between Low Cycles of ALD Films and NMC Cathode Materials Using Molecular Dynamics — ***Julie Nguyen***, *Krishan Kanhaiya, Katarina Odak, Hendrik Heinz, Alan Weimer*
Poster 166d: Sol-Gel Processing of Covalent Organic Frameworks — ***Safiya Khalil***, *Matthew Meyer, Rafael Verduzco*

(167) Poster Session: Materials Engineering & Sciences (08E - Electronic and Photonic Materials)

Monday, Nov 8, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, Exhibit Hall C/D

Matthew Crane, Chair
Evan Wujcik, Co-Chair
Jessica Schiffman, Co-Chair

Sponsored by: Electronics and Photonics

Poster 167a: Design and Optimization of a Tunable Ag-Wire Based Plasmonic Perfect Absorber — ***Alma Vela Ramirez***, *Md Monirul Islam, Andrew C. Hillier*
Poster 167b: Insight into the Reaction Mechanism of Amine Molecules on the Hybrid Halide Perovskite Surface — ***Monimun Nahar Munny***, *Qing Peng*

(168) Poster Session: Materials Engineering & Sciences (08F - Composite Materials)

Monday, Nov 8, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, Exhibit Hall C/D

Kenan Song, Chair
Zhanhu Guo, Co-Chair
Evan Wujcik, Co-Chair
Jessica Schiffman, Co-Chair

Sponsored by: Composites

Poster 168d: Composite CNT-Biopolymer Capacitive Porous Fibers — ***F. John Burpo***, *Enoch Nagelli, Felita Zhang, Alexa S. Zammit, Edward M. Tang, Paul Trackey, Zachary Bone, Malina Hatton*
Poster 168f: Biomineralized Cellulose Acetate Membranes with Strontium Apatite for Guided Bone Regeneration — *Ana Soares, Fabia K. Andrade,****Rodrigo Silveira Vieira***

(169) Poster Session: Nanoscale Science and Engineering

Monday, Nov 8, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, Exhibit Hall C/D

Reginald Rogers Jr., Chair

Sponsored by: Nanoscale Science and Engineering Forum

Poster 169a: Thin Films of Metal Organic Frameworks Interfaces Obtained By Laser Evaporation — ***Olivia Rose***, *Anca Bonciu, Valentina Marascu, Andreea Matei, Qian Liu, Laurentiu Rusen, Valentina Dinca, Cerasela Zoica Dinu*
Poster 169b: *High-Throughput Sonochemical Synthesis of Nanocrystals in Deep Eutectic Solvents* — ***Maria Politi***, *Lilo Pozzo*
Poster 169c: Synthesis of Egyptian Blue and Mechanisms — ***Agoston Kiss***, *Holly A. Stretz*
Poster 169d: Impact of Mesoporous Silica-Encapsulated Gold Core-Shell Nanoparticle Structure on Solvent-Free Aerobic Benzyl Alcohol Oxidation— ***Ellis Hammond-Pereira***, *Steven Saunders*
Poster 169e: Quantitative Spatial Distribution of Rare Earth Dopants in $NaGdF_4$Nanoparticles — ***Ge Zhang***, *Mrinal Bera, Matthew V. Tirrell*
Poster 114h: Gold Nanoparticles Deposited inside Hierarchical Zeolites Catalyze Diverse Groups of Aromatic Alcohols — ***Zengran Sun***, *Steven Saunders*
Poster 169g: COVID-19: Prevent Infection, Diagnosis and Vaccination Using Nanotechnology — *Mahmoud Saeed Mahmoud, Ahmed S. Mahmoud, Areeg M Dabbish,* ***Mohamed Mostafa***, ***Robert Peters***

(170) Poster Session: Novel Products from Forest and Plant Biomass

Monday, Nov 8, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, Exhibit Hall C/D

Xuejun Pan, Chair
Shijie Liu, Co-Chair

Sponsored by: Forest and Plant Bioproducts Division

Poster 170a: *Influence of Dilute Acid Pretreatment and Lignin Extraction Conditions on Lignin and Phenol Formaldehyde Resin Properties* — ***Brian Saulnier***, *Mohsen Siahkamari, Mojgan Nejad, David Hodge*
Poster 170b: Hyrothermal Pyrolysis of Spent Coffee Grounds: Evaluating the Influences of Coffee Roasting Type and Particle Size, and Process Reaction Conditions. — ***Thomas Briscoe***, *Justinus Satrio*
Poster 170c: Fabrication of Hydrogel/Aerogel from Recycled Biomass — ***Mairui Zhang***, *Yang Liao, Gyu Leem, Xuejun Pan, Chang Geun Yoo*
Poster 170d: Assessment of Tribological Properties and Oxidative Stability of Bio-Based Lubricant from Pequi Oil (CARYOCAR BRASILIENSIS) — *Paulo Ribeiro Filho,* ***Francisco Murilo T. Luna***, *Celio Cavalcante Jr.*
Poster 170e: Towards a Sustainable Production of Furfuryl-Alcohol: Conversion of Residual Biomass By Pyrolysis — ***Patricia Hoch***, *Maria Alicia Volpe*
Poster 170f: Effect of Recycling HTC Process Liquid on Hydrochar Morphology and Its Corresponding Performance on Dye Adsorption — ***Md Tahmid Islam***, *Cadianne Chambers, Nepu Saha, Jordan Klinger, Toufiq Reza*

(171) Poster Session: Pharmaceutical Discovery Development and Manufacturing (PD2M)

Monday, Nov 8, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, Exhibit Hall C/D

Andreas Bommarius, Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

Poster 171c: Toxicity of Orally Administered Magnetic Imaging Nanoprobes in an Inflammatory Intestinal Epithelial Cell Model — ***Shno Asad***, *Christel A.S. Bergström, Alexandra Teleki*
Poster 171d: 3D Reporter Gene Assay for High-Throughput Drug Screening— ***You Li***, *Zhen Qin, Shang-Tian Yang*
Poster 171e: Developing Fluorescent Viral Surrogate Particles As an Alternative to Live Virus in Viral Clearance Validation — ***Hannah Doss***, *R. Helen Zha, Todd M. Przybycien*
Poster 171i: Pro-D-Twin: Practitioner Friendly Platform for Process Development, Visibility and Control — ***Ravichandra Palaparthi***, *Jenil Dedhia*

(173) 3D Printing of Composites

Monday, Nov 8, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 202

Mohammad Azad, Chair
Jay Park, Co-Chair

Sponsored by: 3D Printing

3:30 Paper 173a: Deep Composites: Bioinspired AI towards Modeling, Design and Manufacturing — ***Markus J. Buehler***
4:05 Paper 173b: Evaluation of Process Variable Influence on Mechanical Properties of Short Fiber-Reinforced 3D-Printed Parts — ***Martin Etemadi***, *Arit Das, Michael Bortner*
4:28 Paper 173c: Direct Ink Write of High Solid Suspensions: Considerations in Particle Type and Binder Properties — ***Alexandra Marnot***, *Blair Brettmann*
4:51 Paper 173d: Dimensionalization of Two-Phase Newtonian/Non-Newtonian Flow Problems. — ***Abdul Salam Mohammad***, *Joseph J. Biernacki*
5:14 Paper 173e: Influence of Relative Humidity on the Spreadability and Triboelectric Properties of Powders in Additive Manufacturing Processes— ***Sebastien Depaifve***, *Aurelien Neveu, Filip Francqui, Geoffroy Lumay*
5:37 Paper 173f: Toward Next Level of Pharmaceutical 3D-Printing through Advanced Lipid-Based Excipients — ***Moaaz Abdelhamid, MSc***, *Carolina Corzo, Martin Spoerk, Ioannis Koutsamanis, Carolina Alva, Ana Belén Ocampo, Eyke Slama, Dirk Lochmann, Sebastian Reyer, Sharareh Salar-Behzadi*

(174) ABET Updates and Insights (Invited Talks)

Monday, Nov 8, 3:30 PM
Sheraton Back Bay, Republic Ballroom B

Randy Lewis, Chair
Douglas Ludlow, Co-Chair

Sponsored by: Undergraduate Education

(175) Advances in Drug Discovery Processes (including HTE)

Monday, Nov 8, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 101

Luke Rogers, Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

3:30 Paper 175a: Extractionscore: A Quantitative Framework for Evaluating Synthetic Routes on Predicted Liquid-Liquid Extraction Performance — ***Anatoliy Kuznetsov***, *Nikolaos Sahinidis*
3:54 Paper 175b: Accelerating Antibody Discovery with Cell-Free Systems— ***Andrew Hunt***, *Bastian Vogeli, Michael Jewett*
4:18 Paper 175e: A Multiple Molecular Endpoints HT Screening of Embryotoxic Chemicals Based on ESC-EGFP with Human Gene Promoters Associated with Specific Embryonic Development Pathways — ***Fengli Zhang***, *Shang-Tian Yang*
4:42 Paper 175f: Developing a Photonics Platform for Determining Transport Rates of Proton Antiporters — ***Brielle Hohne***, *Manish Kumar*
5:06 Paper 175g: Therapeutically Exploring Persister Metabolism in Bacteria— ***Sayed Golam Mohiuddin***, ***Mehmet Orman***
5:30 Paper 58d: Development of a Novel Continuous Spatially Distributed Diafiltration Unit Operation — ***Xiaoyan Long***, *Zoheb Khan, Eoin Casey, Denis Dowling,* ***Steven Ferguson***

(176) Advances in Process Control II

Monday, Nov 8, 3:30 PM
Sheraton Back Bay, Back Bay Ballroom D

Matthew Ellis, Chair
Joel Paulson, Co-Chair

Sponsored by: Systems and Process Control

3:30 Paper 176a: Development of Algorithms for Reinforcement Learning Augmented Model Predictive Control — ***Elijah Hedrick***, *Katherine Reynolds, Debangsu Bhattacharyya, Stephen E. Zitney, Benjamin P. Omell*
3:49 Paper 176b: Community Detection Based on Dynamic Attributes of Complex Networks — ***Leila Samandari Masooleh***, *Jeffrey E. Arbogast, Ulku Oktem, Warren Seider,* ***Masoud Soroush***
4:08 Paper 176c: On Probabilistic Input Selection: Utilizing a Quantum Algorithm in Selecting Inputs for Lyapunov-Based Economic Model Predictive Control Formulated As a Look-up Table — ***Kip Nieman***, *Keshav Kasturi Rangan, Helen Durand*
4:27 Paper 176d: An Abridged Gaussian Sum Framework to Generalize Extended Kalman Filter for Constrained Nonlinear Systems Under Non-Gaussian Noise — *Mahshad Valipour,* ***Luis Ricardez-Sandoval***
4:46 Paper 176e: Distributed Human-in-the-Loop Model Predictive Control— ***Sambit Ghosh***, *B Wayne Bequette*
5:05 Paper 176f: Statistical Machine Learning in Model Predictive Control of Nonlinear Processes — ***Zhe Wu***, *David Rincon, Panagiotis D. Christofides*
5:24: Break
5:43 Paper 176h: Robust Data-Driven Design of Generic Control Structures with Probabilistic Guarantees Using Gaussian Process Emulators — ***Joel Paulson***, *Ketong Shao, Ali Mesbah*

(177) Applied Artificial Intelligence, Big Data, and Data Analytics Methods for Next-Gen Manufacturing Efficiency II

Monday, Nov 8, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 201

Davood Babaei Pourkargar, Chair

Dimitrios Georgis, Co-Chair

Sponsored by: Next-Gen Manufacturing

3:30: Break
3:50 Paper 177b: Golem: A Probabilistic Approach to Robust Experiment and Process Optimization Based on Regression Trees — ***Matteo Aldeghi***, *Florian Häse, Riley J. Hickman, Isaac Tamblyn, Alán Aspuru-Guzik*
4:10 Paper 177c: Learning Based Scheduling of Industrial Hybrid Renewable Energy Systems — ***P S Pravin***, *Zhiyao Luo, Xiaonan Wang*
4:30: Break
4:59 Paper 177e: Keynote Talk: Modelling and Monitoring with Dynamic Auto-Regressive Latent Variable Methods — ***Qinqin Zhu***, *Bo Xu, Haitian Zhang*

(178) Area Plenary: Fundamentals and Applications of Adsorption and Ion Exchange

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 110

F Handan Tezel, Chair
Peter Ravikovitch, Co-Chair

Sponsored by: Adsorption and Ion Exchange

3:30 Paper 178a: A Review of Common Practices in Gravimetric and Volumetric Adsorption Kinetic Experiments — ***JinYu Wang***, *Enzo Mangano, Stefano Brandani, Douglas Ruthven*
3:50 Paper 178b: Lessons Learnt from over 30 Years of the Zero Length Column Experiment — ***Enzo Mangano***, *Stefano Brandani*
4:10 Paper 178c: A Novel Kinetic Model for the Adsorption Dynamics in Carbon Molecular Sieve and Titanium Silicate Adsorbents — ***Sulaimon Adegunju***, *Armin Ebner, James A. Ritter*
4:30 Paper 178d: Deformation of Amorphous Nanoporous Carbons in the Process of Methane Displacement By Carbon Dioxide — ***Nicholas Corrente***, *Elizabeth Hinks, Alexander Neimark*
4:50 Paper 178f: General Design and Splitting Strategies for Non-Ideal Displacement Chromatography for the Separation of Complex Mixtures — ***Yi Ding***, *Nien-Hwa Linda Wang*
5:10 Paper 178g: Combining Molecular Simulation and Machine Learning to Find Optimal Conditions for Hydrogen Storage and Hydrogen/Nitrogen/Ammonia Separation — *Yangzesheng Sun, Roshan Ashokbhai Patel, Robert DeJaco, Zhao Li, Dai Tang, David Sholl, Coray M. Colina, Randall Snurr, Michael Tsapatsis,* ***Joern Siepmann***
5:30 Paper 178h: Practically Achievable Process Performance Limits for Pressure-Vacuum Swing Adsorption Based Post-Combustion CO_2 Capture.— ***Kasturi Nagesh Pai***, *Vinay Prasad, Arvind Rajendran*
5:50: Break

(179) Biological Catalysis and Enzymatic Catalysis

Monday, Nov 8, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 208

Michael Nigra, Chair
Iman Noshadi, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

3:30 Paper 179a: Enzyme-Based Composites for Next Generation Gas Sensing Platforms. — ***Gia Huy Pham***, *Cerasela Zoica Dinu*
3:55 Paper 179b: Kinetic Modelling of Cephalexin Synthesis By α-Amino Ester Hydrolase (AEH) from *Xanthomonas Campestris Pv. Campestris:* how Substrate Inhibition Affects Reactor Design — ***Colton Lagerman***, *Martha Grover, Ronald Rousseau, Andreas Bommarius*
4:20 Paper 179c: Characterizing Thiamine Diphosphate-Dependent Enzymes for Promiscuous C-C Bond Formation Catalysis — ***Tracey Dinh***, *Bradley W. Biggs, Lindsay Caesar, Paul M. Thomas, Neil L. Kelleher, Linda Broadbelt, Keith Tyo*
4:45 Paper 179d: Combining Oxidases and Metal Nanoparticles for Sequentially Catalyzed Reactions — *Joseph Brindle, Chinmay Verma,* ***Michael Nigra***

(180) Biomass Upgrading II: Novel Catalytic Materials

Monday, Nov 8, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 207

Kenneth Roberts, Chair
Siddarth Krishna, Co-Chair
Jeremy Luterbacher, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

3:30 Paper 180a: Selective Glucose Isomerization to Fructose Using a Heterogeneous Immobilized Tertiary Amine with Tuned Molecular Design— ***Nicholas Brunelli***, *Nitish Deshpande, Li-Chiang Lin, Eun Hyun Cho*
3:48 Paper 180c: Effect of W Dopant on the Hydrodeoxygenation Performance of Mo_2C: Investigating the Microstructure of the Catalyst and Reaction Pathways Using Guaiacol As a Model Compound — ***Sagar Bathla***, *Samir H. Mushrif, Serge Kaliaguine, Chi Cong Tran*
4:06 Paper 180d: Aqueous Phase Hydrogenation of Furfural Using Silica Supported Ultrasmall Bimetallic Catalysts — ***Leandro De Castro***, *Christopher Williams, John R. Regalbuto*
4:24 Paper 53c: Ethanol Oligomerization into Alcohols and Esters over Mg-Al Mixed Oxides Doped with Low-Loadings of Cu — ***Paolo Cuello Penaloza***, *Michael Lanci, Yi Du, George Huber*
4:42: Break
5:00 Paper 180g: Innovative Sol-Gel Routes to Mesoporous Bifunctional Catalysts for the Upgrading of Bioethanol to Butadiene — ***Denis D. Dochain***, *Damien P. Debecker, Ales Styskalik*
5:18 Paper 180h: Morphology Control and Formation Mechanism of Lattice Distortion in Cu-Mn Oxide Catalyst Used in Transfer Hydrogenation of Levulinic Acid — ***Yu Xiao***, *Jinyao Wang, Jiefeng Liu, Wenxiang Zhang, Yiyao Du, Wanqing Li, Changlong Ru, Xin Jin, Chaohe Yang*
5:36 Paper 53f: Deoxygenation of Acetic Acid over Recyclable Mono/Bi/Trimetallic Zeolite Catalysts: Progress Towards Continuous and Scalable Operation — ***James Crawford***, *Jacek Jasinski, Moises A. Carreon*

(181) Biomaterials for Drug Delivery: Nanotechnology Approaches

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 108

Michael Gower, Chair
Rong Yang, Co-Chair
Lisa Volpatti, Co-Chair
Ashish Kulkarni, Co-Chair

Sponsored by: Biomaterials

3:30 Paper 181a: One-Pot Approach for Generating Drug Loaded Nano-Thin Silk Fibroin Coatings for Tissue Engineering Applications — ***Tanner D. Fink***, *R. Helen Zha*
3:48 Paper 181b: Design of a Colloidal Network for Antimicrobial Peptide Protection and Delivery — ***Giovanni Bovone***, *Natthaporn Klubthawee, Ratchaneewan Aunpad, Mark Tibbitt*
4:06 Paper 181c: Stimuli-Responsive, Hydrolysable Layer-By-Layer Nanoparticles Enhance Biofilm Penetration — ***Elad Deiss-Yehiely***, *Paula T. Hammond*
4:24 Paper 181d: Towards Oral Protein Delivery with Poly(acrylamide-co-itaconic acid) Nanoscale Complexation Hydrogels — ***Heidi Oldenkamp***, *Avha R. Mohanty, Nicholas Peppas*
4:42 Paper 181e: Surface Functionalization of Polymer Particles for Cell Targeting By Modifying Emulsifier Chemistry — ***Christopher Isely***, *Kidochukwu Atube, Candice Cheung, Michael Gower*
5:00 Paper 181f: Encapsulation of Salmon Hemoglobin in Silk Nanoparticles for Oxygen Delivery — *Marisa O. Pacheco, Bruce Spiess,* ***Whitney Stoppel***
5:18 Paper 181g: Protein Design Criteria for Intracellular Delivery Via Polyelectrolyte Complex Micelles — *Rachel Kapelner, Justin Horn,* ***Allie Obermeyer***
5:36 Paper 181h: Delivery of HIF1a siRNA for Atherosclerosis Plaques Using Targeted Polyelectrolyte Complex Micelles — ***Ge Zhang***, *Matthew V. Tirrell*

(182) CAST Director's Student Presentation Award Finalists (Invited Talks)

Monday, Nov 8, 3:30 PM
Sheraton Back Bay, Back Bay Ballroom C

Juergen Hahn, Chair
Mona Bavarian, Co-Chair

Sponsored by: Computing Systems and Technology Division

3:30 Paper 182a: Design and Control of Novel Droplet-Based System for Estimating Protein Crystallization Kinetics — ***Moo Sun Hong***, *Amos E. Lu, Jaehan Bae, Jong Min Lee, Richard Braatz*
3:45 Paper 182b: Chemical Representations for Improving Retrosynthesis Prediction: Smiles-Grammar and Information Theory — ***Vipul Mann***, *Venkat Venkatasubramanian*
4:00 Paper 182c: On Representative Day Selection for Capacity Expansion Planning of Power Systems Under Extreme Events — ***Can Li***, *Antonio Conejo, John Siirola, Ignacio Grossmann*
4:15 Paper 182d: Physics-Constrained Deep Learning of Unmodeled Physics in Systems Governed By Stochastic Differential Equations — ***Jared O'Leary***, *Joel Paulson, Ali Mesbah*
4:30 Paper 182e: A Superstructure of Pathways for Pharmaceutical R&D and Its Use in the Optimal Planning of R&D Activities — ***Hua Wang***, *Shekhar Viswanath, Steve Guntz, Jon Dieringer, Shankar Vaidyaraman, Salvador Garcia-Munoz, Chrysanthos Gounaris*
4:45 Paper 182f: Simulation-Optimization Framework for Grey-Box Optimization Using Pharmapy — ***Daniel Laky***, *Daniel Casas-Orozco, Gintaras V. Reklaitis, Carl D. Laird, Zoltan Nagy*
5:00 Paper 182g: Decision-Making Under Epistemic Uncertainty Using Bayesian Hybrid Models — ***Elvis Eugene***, *Xian Gao, Alexander Dowling*
5:15 Paper 182h: Dynamic Trajectory Optimization Via Dynamic Surrogate Modeling — ***William Bradley***, *Fani Boukouvala*

(183) Chemical Recycling of Waste Plastics III

Monday, Nov 8, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 205

Sheima Khatib, Chair
Wan-Ting Chen, Co-Chair
Hilal Ezgi Toraman, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

3:30 Paper 731b: Application of Automatic Fragment Modeling in Plastic Pyrolysis — ***Yen-Ting Wang***, *Matthew Prendergast, William Green*
3:55 Paper 183b: Catalytic Depolymerization of Waste Polyolefins By Induction Heating: Selective Alkane/Alkene Production — ***Bernard Whajah***, *Natalia da Silva Moura, Justin Blanchard, Karleigh Gandar, Scott Wicker, James Dorman, Kerry M. Dooley*
4:20 Paper 183c: Low-Temperature, Energy-Efficient Hydrocracking of Polyolefins to Fuels — ***Pavel Kots***, *Sibao Liu, Brandon Vance, Dionisios Vlachos*
4:45 Paper 183d: Understanding Chemical Recycling of Step-Growth Polymers Using Kinetic Monte Carlo Approach — ***Gorugantu SriBala***, *Ana R. C. Morais,*

Nicholas A. Rorrer, Bonnie L. Buss, Gregg T. Beckham, Robert D. Allen, Linda Broadbelt
5:10 Paper 183e: Targeting Fuel-Ranged Aromatics through Co-Pyrolysis of Polystyrene and Polyethylene with H-ZSM5 — ***Thang Luong**, Changle Jiang, Yuxin Wang, Jianli Hu*
5:35 Paper 183f: Synergetic Effects of Co-Pyrolysis of Hdpe and Various Biomass Feedstocks By ZSM-5 and MCM-41/ZSM-5 Composites — ***Jeffrey Page**, Lei Yu, Azeem Farinmade, Oluwole Ajumobi, Vijay T. John, Julia A. Valla*

(184) Conceptual Process Design and Operational Improvements in Refining, Petrochemicals and Gas Processing

Monday, Nov 8, 3:30 PM
Marriott Copley Place, Fairfield

Nevin Gerek Ince, Chair
Ian Boys, Co-Chair
Vladimir Mahalec, Co-Chair
Helen Lou, Co-Chair

Sponsored by: Fuels and Petrochemicals Division

3:30 Paper 184a: Microwave-Assisted Demulsification of Tight Crude Oil-Water Emulsions — ***Prasad Pawar**, Pankti Joshi, Clayton Jeffryes*
3:45 Paper 184d: Optimal Control for Pipeline Flushing Operations in Lubricants Blending and Packaging Industries — ***Swapana Jerpoth**, Robert Hesketh, Mariano J. Savelski, C. Stewart Slater, Robert McClernan, Kirti Yenkie*

(185) Continuous Drug Product

Monday, Nov 8, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 102

Nicholas Vecchiarello, Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

3:30 Paper 58f: Flow Chemistry As an Enabling, Green Technology in Merck Process — ***Karthik Narsimhan**, Michael Di Maso, Francois Levesque, Jeffery Kuethe, Jacob H. Forstater, Christopher Prier, Nadine Kuhl, Brian Wyvratt, Jonathan McMullen, Matthew Burris, Ji Qi, Gao Shang, Karla Camacho Soto*
3:54 Paper 58e: Impurity Purging through Systematic Process Development of a Continuous Two-Stage Crystallization — ***Michael Scott**, Naomi Briggs, Thomas Roper*
4:18 Paper 185c: Non-invasive, continuous, quantitative detection of powder level, mass holdup and moisture fraction in pharmaceutical GMP vessels— ***Michel Louge**, Robert F. Meyer, Jasdeep Mandur, William Blincoe, Anthony Tantuccio*
4:42 Paper 185e: Residence Time Distribution (RTD) Study of Chute Transition Zones between Unit Operations — ***Jingzhe Li**, James Scicolone, Sonia M. Razavi, Andres Roman-Ospino, Carlos Ortega-Zuniga, Marianthi Ierapetritou, Fernando Muzzio*
5:06 Paper 185g: Adaptive Nonlinear Model Predictive Control of a Continuous Direct Compaction Tablet Manufacturing Process — ***Yan-Shu Huang**, M.Ziyan Sheriff, Sunidhi Bachawala, Marcial Gonzalez, Zoltan Nagy, Gintaras V. Reklaitis*

(186) Data-Driven Design and Modeling II

Monday, Nov 8, 3:30 PM
Marriott Copley Place, Salon J/K

Stephanie Valleau, Chair
Qing Shao, Co-Chair
Yi He, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

3:30 Paper 186a: Automated Solid State Electrolyte Conductivity Predictions Via Probability Density Analysis — ***Karun Kumar Rao**, Yan Yao, Michael Nikolaou, Christopher M. Wolverton, Lars Grabow*
3:45 Paper 186c: Bayesian Model Selection: Applying Parsimony to Build Better Molecular Models — ***Owen Madin**, Simon Boothroyd, Richard A. Messerly, Michael Shirts*
4:00 Paper 186d: Addressing Well-Posedness in a Data-Driven Manner: Model Problems and Physics-Informed Neural Networks — ***Thomas Bertalan**, George Kevrekidis, Siddhartha Mishra, Ioannis G. Kevrekidis*
4:15 Paper 186e: Evaluating Polymer Stabilizer Performance Using Molecular Descriptors and Machine Learning on a Small Dataset — ***Aaron Liu**, Rahul Venkatesh, Michael McBride, Elsa Reichmanis, J Carson Meredith, Martha Grover*
4:30 Paper 186f: Machine-Learning-Guided Discovery of New Electrochemical Reactions — ***Andrew Zahrt***
4:45 Paper 186g: A Deep Learning Potential to Study Large-Scale Anhydrous Proton Transport Systems — ***Siddarth Achar**, Linfeng Zhang, Leonardo Bernasconi, Karl Johnson*
5:00 Paper 186h: Leveraging Machine Learning Techniques to Identify Ionic Liquids Possessing High Ionic Conductivity — ***Pratik Dhakal***
5:15 Paper 186j: High-Throughput Electrochemical Screening of Deep Eutectic Solvents for Use in Redox Flow Batteries — ***Maria Politi**, Jaime Rodriguez Jr., Lilo Pozzo*
5:30 Paper 707f: Deep Learning for Morphology Detection of Self-Assembled Oligomers in Atomistic Simulations: Pointnet — ***Zhengyuan Shen**, Yangzesheng Sun, Ke Luo, Mahesh Mahanthappa, Timothy P. Lodge, Joern Siepmann*

(187) Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains III

Monday, Nov 8, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 313

Dharik Mallapragada, Chair

Sponsored by: Sustainable Energy

3:30 Paper 187a: Design and Optimization of a Sustainable Beccs Supply Chain in the European Union to Reduce the Stress on Core Planetary Boundaries — ***Valentina Negri**, Gonzalo Guillén-Gosálbez*
3:55 Paper 187b: Techno-Economic Evaluation of Manure Pre-Treatment Strategies for the Production of Biogas — *Yicheng Hu, Joonrae Kim, Krishnapuram Karthikeyan, **Victor M. Zavala***
4:20 Paper 187c: Modeling and Designing Renewable Energy Systems in Rural Areas with Flexible Operating Units — *Andras Eles, Istvan Heckl, **Heriberto Cabezas***
4:45 Paper 187d: Analysis of Marginal Land Definition on Integrated Landscape Design and Biofuel Supply Chain Network Design Optimization — ***Eric O'Neill**, Rafael Martinez-Feria, Tyler Lark, G. Philip Robertson, Bruno Basso, Christos Maravelias*
5:10 Paper 187e: Economic Analysis Linking Fuel Property to Potential Value of Diesel-Boiling-Range Bio-Blendstocks to Petroleum Refiners — ***Yuan Jiang**, Shuyun Li, Avantika Singh, Nicholas Carlson, Michael Talmadge, Daniel J. Gaspar*

(188) Developments in Extractive Separations: Processes

Monday, Nov 8, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 108

George S. Goff, Chair
David Cantu, Co-Chair

Sponsored by: Extractions

3:30 Paper 188a: Phase Separation Kinetics in Liquid-Liquid Extraction and Settler Design — *Pornprapa Bol, Georg Rudelstorfer, Jan Bernd Bol,**Matthaeus Siebenhofer**, Annika Grafschafter*
4:00 Paper 188b: Three Phase Flow and Four Phase Flow in the Taylor Couette Disc Contactor for Combination of Liquid-Liquid Extraction and Chemical Reaction — ***Georg Rudelstorfer**, Susanne Lux, Matthaeus Siebenhofer, Annika Grafschafter*
4:30 Paper 188c: New Developments in Membrane Solvent Extraction — ***Lydia Rodrigues**, Kamalesh Sirkar, Kirk R. Weisbrod, John C. Ahern, Uwe Beuscher*
5:00 Paper 188d: Oil Recovery from Dilute Oil-Water Mixtures Via Hydrophobic Hollow Fiber Membranes — ***Carolyn Cooper**, Lynn E. Katz, Kerry Kinney, Albert Seibert*
5:30 Paper 188e: Cellulose Nanocrystals- and Lignin Magnetic Nanocomposites Enhance the Ethanol Extraction from Aqueous Solution Using Castor Oil As the Extractant — ***Peng Chen**, Mohammad Jahid Hasan, Abhishek Saini, Sarah J. Watzman, Esteban E. Urena-Benavides, **Erick Vasquez***

(189) Distillation and Absorption Processes Fundamentals, Developments, Optimization, and Applications

Monday, Nov 8, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 109

Tony Cai, Chair
Gregory A. Cantley, Co-Chair

Sponsored by: Distillation and Absorption

3:30: Break
4:00 Paper 189b: Design of Gas Separation Processes Using Type II Porous Liquids As Physical Solvents — ***Isaiah Borne**, Natalie Simon, Christopher W. Jones, Ryan Lively*
4:30 Paper 189c: Separation of Azeotropic Refrigerant Mixtures Using Extractive Distillation with Ionic Liquid Entrainers — ***Ethan Finberg**, Kalin Baca, Abby Harders, Andrew Yancey, Mark Shiflett*
5:00: Break
5:30 Paper 189f: Separation of Complex Mixture and Solvent Recylcing Using Dividing Wall Batch Column — ***Urmila Diwekar**, Rakesh Agrawal*

(190) Electrocatalysis and Photoelectrocatalysis IV: Hot Topics

Monday, Nov 8, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 204

Linsey Seitz, Chair
Omar Abdelrahman, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

3:30 Paper 237c: Single Metal Atom in N Doped Graphene for Electrocatalytic CO2 and Oxygen Reduction: Activation Energies and Catalytic Mechanisms— ***Yuanyue Liu***
3:48 Paper 190b: Revised Activity Descriptor for Recombinative Hydrogen Desorption — ***Chenghao Wang**, Lars Grabow*
4:06 Paper 190c: Catalyst Design Strategies for the Alkaline Hydrogen Evolution Reaction — ***Ian McCrum***
4:24 Paper 190d: Unifying Concepts in Electro- and Thermocatalysis Towards Hydrogen Peroxide Production — ***Jason Adams**, Matthew Kromer, Joaquín Rodríguez-López, David Flaherty*
4:42 Paper 509aq: Degradation Mechanisms of Calcium Iridium Oxides for Oxygen Evolution Reaction in Acid — ***Ruihan Li**, Linsey Seitz*
5:00 Paper 190f: Mechanisms of Proton-Coupled Electron Transfer at Electrochemical Interfaces — ***Robert Warburton**, Phillips Hutchison, William Lake, Alexander Soudackov, Sharon Hammes-Schiffer*
5:18 Paper 190g: Correlating Atomic-Scale Compositions and Structures of Mesoporous N-Containing Carbon Electrocatalysts with Oxygen and Sulfur Reduction Properties — ***Shona Becwar**, Ziyang*

Wei, Rongli Liu, Walter Rosas, Anders Palmqvist, Xiangfeng Duan, Bradley F. Chmelka
5:36 Paper 190h: Additive Manufacturing of Digitally Optimized Porous Electrodes for Enhanced Energy Efficiency — ***Jonathan Davis**, Buddhinie Jayathilake, Tiras Lin, Swetha Chandrasekaran, Joshua R. DeOtte, Jonathan M. Wong, Sarah Baker, Victor Beck, Eric B. Duoss*

(191) Electrochemistry and Electrocatalysis

Monday, Nov 8, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 206

Elizabeth Biddinger, Chair
Fanglin Che, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

3:30 Paper 237b: Oxygen Electrocatalysis on Two-Dimensional Graphene or Hexagonal Boron Nitride Materials — ***Drew Higgins***
4:00 Paper 191b: The Active Structure of Single Nickel Atom in Graphene for Electrocatalytic CO2 Reduction — ***Yuanyue Liu***
4:18 Paper 191f: Investigating Mixed Metal Oxides As Cathode Electrocatalysts for CO_2 reduction in Solid Oxide Electrolysis Cell — ***Elif Tezel**, Ariel Whitten, Reinhard Denecke, Jean-Sabin McEwen, Eranda Nikolla*
4:36 Paper 509ak: CO2RR-to-C2 Enhanced By Confined Organic-Inorganic Interface — ***Mingyu Wan**, Zhiyong Gu, Fanglin Che*
4:54 Paper 191a: Revisiting Electrochemical CO_2 Reduction on Copper: Reaction Mechanisms Revealed By Embedded Correlated Wavefunction Theory— ***Qing Zhao**, John Mark P. Martirez, Emily A. Carter*
5:12 Paper 237e: Promoting H_2O_2 Production Via 2-Electron Oxygen Reduction By Coordinating Partially Oxidized Pd with Defect Carbon — ***Amir Hassan Bagherzadeh Mostaghimi**, Zheng Chen, Samira Siahrostami, Qiaowan Chang, Pu Zhang, Steven R. Denny, Ji Hoon Lee, Hongpeng Gao, Ying Zhang, Huolin L. Xin, Jingguang G. Chen*
5:30 Paper 237f: From First-Principles Calculations to Data-Driven Discovery and Materials Design of Mxene Electrocatalysts — ***Luke Johnson**, Brandon Burghardt, Yamilée Morency, Aleksandra Vojvodic*

(192) Faculty Candidates in COMSEF/Area 1a, Session 2

Monday, Nov 8, 3:30 PM
Marriott Copley Place, Salon A/B

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

Sponsored by: Thermodynamics and Transport Properties

3:30 Paper 192a: Bridging Homogenous and Heterogenous Catalysts: Computational Design of Catalysts at Atomic Scale — ***Mingjie Liu***
3:42 Paper 192b: First-Principles Design of Heterogeneous Catalysts with Automatic Simulations — ***Daniel Schwalbe-Koda***
3:54 Paper 192c: Two-Dimensional Energy Histograms As Features for Machine Learning to Predict Adsorption in Metal-Organic Frameworks— ***Kaihang Shi**, Zhao Li, Randall Snurr*
4:06 Paper 192d: Disordered Hyperuniform Networks and Their Application in Atomic-Scale Low-Dimensional Materials — ***Duyu Chen***
4:18 Paper 192e: Machine Learning-Directed Advanced Sampling Simulations of Reactions in Condensed Phases — ***Elizabeth M.Y. Lee**, Guilia Galli, Juan J. de Pablo*
4:30 Paper 192f: Development and Implementation of Enhanced Sampling Approaches: Applications to Ion-Pairing in Battery Electrolytes and Nucleation of Nano-Porous Materials — ***Ajay Muralidharan**, J.R. Schmidt, Arun Yethiraj*
4:42: Break
5:07 Paper 192h: What Is a "Hydrophobic" Solute? a Detailed Examination of Driving Forces for Adsorption of Small, Neutral Solutes at Chemically Patterned Interfaces — ***Jacob I. Monroe**, Sally Jiao, R. Justin Davis, Dennis Robinson Brown, Lynn E. Katz, M. Scott Shell*
5:19 Paper 192i: Data-Driven Design of Solid-State Electrolytes — ***Karun Kumar Rao***
5:31 Paper 192j: Generating Molecules with Optimized Solubility Using Iterative Graph Translation — ***Camille Bilodeau**, Sukrit Mukhopadhyay, Jillian Emerson, Hongyun Xu, Wengong Jin, Regina Barzilay, Klavs F. Jensen*
5:43 Paper 192k: Leveraging Thermodynamic Calculations Towards Predictive Solid-State Materials Synthesis — ***Christopher J. Bartel**, Akira Miura, Wenhao Sun, Gerbrand Ceder*

(193) Feedstock Logistics for Biorefineries

Tuesday, Nov 16, 3:30 PM
Virtual, Sustainable Engineering Forum (23)

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

Sponsored by: Sustainable Biorefineries

3:30: Break
3:51 Paper 193b: Combined Alkali Treatment and Anaerobic Storage in Corn Stover Enhances Reactivity and Surface Energy Properties — ***Lynn Wendt**, Bradley Wahlen, Troy Semelsberger, Juan Leal, Corey Pilgrim, Michelle Walton*
4:12 Paper 193c: Air-Classification of Forest Residues for Beneficiated High Temperature Conversion Feedstock — ***Jordan Klinger**, Neal Yancey, Rachel Emerson, Yidong Xia, Tiasha Bhattacharjee, Susan Carilli, Vicki Thompson*
4:33 Paper 193d: Population Balance of Knife Milled Corn Stover — ***Tiasha Bhattacharjee**, Jordan Klinger, Susan Carilli, Vicki Thompson, Neal Yancey*
4:54 Paper 193e: Simulating the Operational Effect of Particle Scale Impacts on Deconstruction Energy of Pine Residues. — ***Damon Hartley**, David Thompson, Matthew Wiatrowski, Abhijit Dutta*
5:15 Paper 193f: Optimal Depot Size and Location Selection in Biofuel Supply Chain Under Temporal and Spatial Variabilities over a 10-Year Period— ***Yingqian Lin**, Roni Mohammad, David Thompson, Damon Hartley*
5:36 Paper 193g: Nuclear Powered Biorefineries: A Nationwide Supply Chain Analysis — ***Tasmin Hossain**, Daniela Jones, Charles Forsberg, Bruce Dale, Lynn Wendt*

(194) Fluidization: Industrial Application of Computational and Numerical Approaches to Particle Flow & Cohesive Materials

Monday, Nov 8, 3:30 PM
Sheraton Back Bay, Fairfax A/B

Michael Molnar, Chair
Andrew P. Santos, Co-Chair
Reza Mostofi, Co-Chair
Fanxing Li, Co-Chair

Sponsored by: Fluidization and Fluid-Particle Systems

3:30 Paper 194b: CFD Modeling and Liquid Vaporization: Industrial FCC Riser Feed Injection Application — ***Peter Blaser**, Ali Akhavan*
3:49 Paper 701b: Machine Learning Based Interaction Force Model for Non-Spherical Particles in Incompressible Flows — ***Soohwan Hwang**, Jianhua Pan, L.-S. Fan*
4:08 Paper 194c: Experiments and Simulations of Gas-Solid Flow Dynamics with a Moving Porous Media Model — ***Julia Hartig**, Davis R. Conklin, Alan Weimer*
4:27 Paper 194d: Optimization of Fluidized Bed Incineration Process for Explosive Waste Treatment Via Artificial Neural Network Surrogate Modeling Method — ***Sunghyun Cho**, Minsu Kim, Hyungtae Cho, Junghwan Kim, Il Moon*
4:46 Paper 194e: Numerical Analysis and Experimental Verification of Boehmite to Alumina Particles Conversion Under Concentrating Light — ***Konstantinos E. Kakosimos**, Fathya Salih, Navaira Fathima, Mamoun Al-Rawashdeh, Athanasios G. Konstandopoulos*
5:05 Paper 194f: Extraction of Particle-Scale Cohesion Parameters from Straightforward Bulk Measurements — ***Ipsita Mishra**, Abhishek Shetty, Christine Hrenya*
5:24: Break

(195) Fluid Mechanics Poster Session

Monday, Nov 8, 3:30 PM
Sheraton Back Bay, Constitution A

Anthony Kotula, Chair
Vivek Narsimhan, Co-Chair

Sponsored by: Fluid Mechanics

Poster 195a: Characterizing the hMSC-Mediated Remodeling of Polymer-Peptide Hydrogels on Multiple Length Scales Using Bi-Disperse Multiple Particle Tracking Microrheology — ***John McGlynn**, Kilian J. Druggan, Kiera J. Croland, Kelly Schultz*
Poster 195b: Structural Instability and Transport of Flexible Fibers with Non-Uniform Rigidity — ***Thomas Minh Nguyen**, Harishankar Manikantan*
Poster 195c: Learning Physically Informed Differential Viscoelastic Constitutive Models from Data — ***Kyle Lennon**, James Swan*
Poster 195d: Testing the Effectiveness of Free-Standing Hepa Filters Placed in Operating Rooms to Reduce the Spread of Contaminated Particles Using Computational Fluid Dynamics — ***Mahir Alam**, Emily Yasharpour, Mitchell Weiser, Jennifer Weiser*
Poster 195e: Numerical Simulation of Acoustic Streaming Flows in Non-Newtonian Fluids — *Beijia Yao, Vijay K. Gupta, Md. Rifat Hassan, Cheng Wang,* ***Joontaek Park***
Poster 195f: Frequency Dependence of Ionic Conductivity in Concentrated Electrolytes — ***Emily Krucker Velasquez**, James Swan*
Poster 195g: Rheology and Behavior of Wormlike Micelles: Using Neutron Scattering and Specific Salt Interactions to Understand the Onset of Shear Alignment — ***Nour Alawami**, Javen Weston*
Poster 195h: Characterizing Rheological Properties for Both Polydisperse and Monodisperse Colloidal Rod Systems — ***Shiqin He**, Dominic Pascucci, Marco Caggioni, Seth Lindberg, Kelly Schultz*
Poster 195i: Instabilities in the Flow Around a Rotating Finite-Size Disk— ***Ziyao Liu**, Tony Ladd*
Poster 195j: Dissolution of a Single Disk: Validation and Refinement of Pore-Scale Simulations — ***Liang Yu**, Tony Ladd, Piotr Szymczak*
Poster 195k: Interfacial Flows and Instabilities of Boger Fluids — ***Fahed Albreiki**, Alexander Kubinski, Andrew Rasmussen, Jelena Dinic, Vivek Sharma*
Poster 195l: The Kitchen Pot Thickens, Drop By Drop — ***Karthika Suresh**, Lena Hassan, Chenxian Xu, Michael Boehm, Stefan Baier, Vivek Sharma*
Poster 195m: Macromolecular Engineering of Rheology and Pinching Dynamics of Formulations — ***Chenxian Xu**, Vivek Sharma*
Poster 195n: Influence of Surfactants, Polymers and Proteins on Foam Film Drainage — ***Chenxian Xu**, Lena Hassan, Chrystian Ochoa, Vivek Sharma*
Poster 195o: Confinement and Wettability Effects on the Observed Rheology in Microcapillary Flow — ***Javen Weston**, Elio Trigo, Amita Kosambi*
Poster 195p: Optimal Control of Active Liquid Crystals — ***Michael Norton**, Piyush Grover, Michael F. Hagan, Seth Fraden*
Poster 195q: Sorting Red Blood Cells (RBCs) By Deformability in a Microfluidic Device — ***Luca Brandt***

(196) Free Forum on Engineering Education: Special Topics, Unique Modules, and Research-Based Electives

Monday, Nov 8, 3:30 PM
Sheraton Back Bay, Liberty B/C

Sandra Pettit, Chair
Michael Elsass, Co-Chair
Courtney Pfluger, Co-Chair

Sponsored by: Undergraduate Education

3:30 Paper 196a: Bourbon Production Engineering: Teaching Cheme Concepts to Anyone through the Science of Bourbon — *Brad J. Berron, Anastasia K. Hauser,* ***Sarah Wilson***
3:48 Paper 196b: Re-Envisioning a Faculty-Led, International, Chemical Engineering Experiential Program in a Virtual Format — ***Courtney Pfluger***
4:06 Paper 196c: A Sustainability and Alternative Energy Course As a Bridge between Disciplines — ***Benjamin Davis****, Amanda Simson*
4:24 Paper 196d: Even More Steal-Able: Thermodynamics Concept Laboratories & Projects — ***Margot Vigeant***
4:42 Paper 196e: Using Social Frameworks and Trusted Influencers to Mediate Inter-Generational Conflicts over Social Justice in the Classroom — ***Peter J. Ludovice***
5:00: Break
5:18: Break
5:36 Paper 196h: Teaching Principles of Biomaterials during the COVID-19 Pandemic with at-Home Inquiry-Based Learning Laboratory Experiments— ***Chris Panebianco****, James Iatridis, Jennifer Weiser*

(197) Graduate Student Competition in Microbiointerface Research

Monday, Nov 8, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 310

Huan Gu, Chair
Fangchao Song, Co-Chair

Sponsored by: Microbes at Biomedical Interfaces

3:30 Paper 197a: The Triggered Delivery of Polymyxin Antibiotics from Polyelectrolyte Microgels — ***Xixi Xiao****, Jingjing Ji, Wenhan Zhao, Shikha Nangia, Matthew Libera*
3:48 Paper 197e: Advancing the Functionality of Dimethylallylamine-Based Nanocultures for Selective Transport and Controlled Microbial Dynamics.— ***Shanna-Leigh Davidson****, Tagbo H. R. Niepa, PhD*
4:06 Paper 197c: Biofilm Reduction Via Surface Vs. Immersion Heating— ***Parham Parnian****, Paraskevi Konstantina Zoga, Haydar Aljaafari, Jaymes Van Dyne, Eric Nuxoll*
4:24 Paper 197b: A New Antimicrobial Peptide-Antibiotic Combination Strategy for *P. Aeruginosa* Inactivation — ***Wenxu Han****, Terri A. Camesano*
4:42 Paper 197g: A Targeted Genome-Wide Approach to Elucidate and Control Bacterial Adhesion to Physicochemically Diverse Biomaterials — ***Stephanie Call****, Brandon Ugbesia, Vanessa Vu, Lauren B. Andrews*
5:00 Paper 197f: Establishing Relationships between Local pH and Mechanics in *Staphylococcus Epidermidis* Biofilms — ***Patryck Michalik****, Elizabeth Stewart*
5:18 Paper 197d: Design of a Well-Defined Poly(dimethylsiloxane)-Based Microbial Nanoculture System — ***Huda Usman****, Tagbo H. R. Niepa, PhD*
5:36 Paper 197h: To Biofilm or Not to Biofilm: Interplay between Chemotactic Dispersal and Biofilm Formation in Bacterial Communities — ***Jenna Ott****, Daniel B. Amchin, Selena Chiu, Tapomoy Bhattacharjee, Sujit Datta*

(198) Green Chemistry and Engineering-I

Monday, Nov 8, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 311

Lindsay Soh, Chair
Christina Tang, Co-Chair
Wenqin Li, Co-Chair

Sponsored by: Sustainability Science and Engineering

3:30 Paper 198a: Replacement of Fluorinated Aqueous Fire-Fighting Foams (AFFF) — ***William Barrett***
3:50 Paper 198c: Green and Sustainable Processes for Critical Metal Recovery Using Oxalate Chemistry — ***Ankit Verma****, Alexander J. Henne, David R. Corbin, Mark Shiflett*
4:10 Paper 198e: Evaluating Green Solvent Nanoparticle Production Via Supercritical Fluid Synthesis — ***Mary Kate Lane****, Julie B. Zimmerman*
4:30 Paper 198f: Green Solvent Selection Using End-of-Life Metrics — ***Lindsay Soh****, Sasha Neefe*
4:50 Paper 198g: Emergy and SPI Assessment of Solvent Recovery Pathways— ***Emmanuel A Aboagye****, John Chea, Austin Lehr, Jake Stengel, Kayla Heider, C. Stewart Slater, Mariano J. Savelski, Kirti Yenkie*

(199) Honorary Session for Prof. Andrew Zydney II

Monday, Nov 8, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 304

Ying Li, Co-Chair
Ehsan Espah Borujeni, Co-Chair
Mahsa Rohani, Co-Chair

Sponsored by: Membrane-Based Separations

3:30 Paper 255d: Zydney Abstract 4 — ***Hari Pujar***
3:50 Paper 199d: Bioinspired Ideas for Sustainable Separations — ***Manish Kumar***
4:10 Paper 255c: Zydney Abstract 3 — ***Hasin Feroz***
4:30 Paper 131f: Flow Distribution in Commercial Depth Filter Capsules for Clarification of Cell Culture Fluid – Effects on Performance and Scale-up— ***Negin Nejatishahidein****, Minyoung Kim, Lara Fernandez Cerezo, Ehsan Espah Borujeni, David Roush, Ali Borhan, Andrew Zydney*
4:50 Paper 199b: Understanding Prefiltration and Fouling of Virus Filters — *Solomon Isu, Ranil Wickramasinghe, Andrew Zydney,* ***Xianghong Qian***
5:10 Paper 199c: A Stand-Alone Evapoporometer for Determining the Pore-Size Distribution of Membranes and Other Porous Media — ***William Krantz****, Michael Dy Cham Lua, Jose Luy Absalon, Babu Narayanswamy*
5:30 Paper 255e: Ultrafiltration membranes on the purification of plasmid DNA templates for mRNA vaccines — ***Ivan Manzano****, Marcus Duvall, Jason Murphy*

(200) In Honor of the Chemical Engineering Professor Amyn Teja (Invited Talks)

Monday, Nov 8, 3:30 PM
Marriott Copley Place, Salon C/D

Ronald Rousseau, Chair

Sponsored by: Thermodynamics and Transport Properties

3:30 Paper 200a: What Do We Really Know about Mixture Adsorption?— ***David Sholl***
3:55 Paper 200c: The Role of Interfacial Properties in Gas Hydrate Energy & Carbon Capture Applications — ***Carolyn Koh***
4:20 Paper 200b: Peptide Co Assembly--a New Frontier in Biomaterials— ***Carol Hall***

(202) In Honor of William M. Deen (Invited Talks)

Monday, Nov 8, 3:30 PM
Sheraton Back Bay, Independence Ballroom East

Sara Hashmi, Chair

Sponsored by: Transport Processes

3:30 Paper 202a: Honoring Bill Deen: Analytical Simplifications in Transport Fundamentals — ***Sara Hashmi***
3:45 Paper 202b: Time and Length Scales for Hypoxia-Mediated Cell Signaling in Pancreas Cancer — ***Matthew Lazzara***
4:00 Paper 202c: Mechanistic Modeling of the Loss of Protein Sieving Due to Internal and Externalfouling of Microfilters — ***Glen Bolton****, Alex Apostolidis*
4:15 Paper 202d: Analyzing Transport Phenomena in the Kidney — ***Aurelie Edwards***
4:30 Paper 202e: Enabling Accelerated Downstream Process Development for Diverse Protein Therapeutic — ***Chen Wang***
4:45 Paper 202f: Analysis of Transport Phenomena: The Legacy of Bill Deen in 10.50 — ***Martin Z. Bazant***
5:00 Paper 202g: Lessons I Learned — ***Behrooz Satvat***
5:15 Paper 202i: A Journey in Research- Coming Full Circles — ***Randy Lewis***
5:30 Paper 202h: Honoring Bill Deen — ***Kim Kosto***
5:45 Paper 202j: Honoring Bill Deen - Kristin Mattern — ***Kristin Ploeger***

(203) Innovations in Methods of Data Science

Monday, Nov 8, 3:30 PM
Marriott Copley Place, Salon H/I

Andrew White, Chair
Srinivas Rangarajan, Co-Chair

Sponsored by: Applications of Data Science to Molecules and Materials

3:30 Paper 203a: The Euler Characteristic: A General Topological Descriptor for Complex Data — ***Alexander Smith****, Victor M. Zavala*
3:45 Paper 203b: Machine Learning + Automated Reasoning for Theory Discovery — ***Tyler Josephson****, Vernon Austel, Kenneth A. Clarkson, Cristina Cornelio, Sanjeeb Dash, Bachir El Khadir, Joao Goncalves, Lior Horesh, Sharon Liu, Nimrod Megiddo, Francesca Nacion, Neil Tran, Catherine M. Wraback*
4:00 Paper 203c: Characterizing Uncertainty and Error in Machine Learning Chemical Property Prediction — ***Esther Heid****, Charles J. McGill, Florence Vermeire, William Green*
4:15 Paper 203d: Giving Attention to Generative Models for *De Novo M*olecular Design — ***Orion Dollar****, Nisarg Joshi, David Beck, Jim Pfaendtner*
4:30 Paper 203e: Improving Data Sub-Selection for Supervised Tasks with Principal Covariates Regression — ***Rose Cersonsky****, Benjamin Helfrecht, Sergei Kliavinek, Edgar A. Engel, Michele Ceriotti*
4:45 Paper 203f: Chemical Identification in Multicomponent Electrolytes Using Voltammetry, Physics-Based Modeling, and Bayesian Inference — ***Alexis Fenton Jr.****, Fikile R. Brushett*
5:00: Break
5:15 Paper 203h: Deep Learning-Assisted Analysis of Anomalous Nanoparticle Surface Diffusion in Liquid Phase Transmission Electron Microscopy — ***Vida Jamali****, Cory Hargus, Assaf Ben-Moshe, Hyun Dong Ha, Kranthi K. Mandadapu, A. Paul Alivisatos*
5:30 Paper 203i: A Principal Component Normalizing Flow for Modeling Renewable Electricity Generation — ***Eike Cramer****, Alexander Mitsos, Manuel Dahmen*

(204) Intellectual Property for Practicing Engineers: Patents and Trade Secrets

Wednesday, Nov 17, 12:30 PM
Virtual, Chemical Engineering & the Law Forum (24)

Paul Townsend, Chair
Charles Collins-Chase, Co-Chair
Lauren Dowty, Co-Chair

Sponsored by: Chemical Engineering & the Law Forum

12:30 Paper 204a: Intellectual Property and Carbon Capture — ***Paul Townsend****,* ***Lauren Dowty****, Charles Collins-Chase*
12:45 Paper 204b: Green Technology: Innovation and Regulatory Trends— ***Matthew Zapadka***

1:00 Paper 204c: Patent Ownership and Inventorship Considerations in Collaborations — ***Andrew Renison***

(205) Modeling and Control of Crystallization

Monday, Nov 8, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 302

Zoltan Nagy, Chair
Yamil Colón, Co-Chair

Sponsored by: Crystallization and Evaporation

3:30: Welcoming Remarks
3:33 Paper 205a: Modeling Impurity-Mediated Crystal Growth — ***Tobias Mazal***, *Michael F. Doherty*
3:54 Paper 205b: Combination of in Situ Imaging and Deep Learning for Crystallization Process Monitoring: Application to Beta-Lactam Antibiotics Manufacturing — ***Hossein Salami***, *Matthew McDonald, Andreas Bommarius, Ronald Rousseau, Martha Grover*
4:15 Paper 205c: Brownian Dynamics Simulations Predict the Nucleation Probability of Polymorphs during the Process of Crystallization — ***Anish Dighe***, *Prem Kumar Reddy Podupu, Paria Coliaie, Meenesh Singh*
4:36 Paper 205d: Kinetic Monte Carlo Modeling of MIL-53 Metal Organic Framework Crystal Growth — ***Andrew Garcia***, *Janani Sampath, Sergey Vasenkov, Kirk J. Ziegler*
4:57 Paper 205e: Digital Twin Design of an Agrochemical Crystallization Process Using a 2D Population Balance Model Approach — ***Wei-Lee Wu***, *Chris Chappelow, Madhusudhan Kodam, Paul A. Larsen, Patrick McGough, Jasson T Patton, Aaron A. Shinkle, Zoltan Nagy*
5:18 Paper 205f: Optimization of Energetics Crystallization Via Quality-By-Control Direct Design Approaches — ***Montgomery Smith***, *Wei-Lee Wu, Daniel Laky, Jaron Mackey, Zoltan Nagy*

(206) Novel Nanoparticles and Nanostructured Catalysis for Energy and Environmental Applications

Monday, Nov 8, 3:30 PM
Sheraton Back Bay, Hampton

Timothy M. Brenza, Chair

Sponsored by: Nanoparticles

3:30 Paper 206a: Flame Aerosol Synthesis of Mesoporous Silica for Application in CO_2 Oxidative Dehydrogenation of Propane — ***Shuo Liu***, *Junjie Chen, Satyarit Rao, Mihir Shah, Abhishek Kumar, Eleni Kyriakidou, Mark Swihart*
3:45 Paper 206b: Role of Water in Methane Oxidation Observed By Transient Drifts at Low Temperatures Using Bimetallic Aupd Catalysts — ***Joseph Brindle***, *Michael Nigra*
4:00 Paper 206d: Continuous Green Millifluidic Synthesis of Five-Fold Palladium Nanorods Using L-Ascorbic Acid and Their Catalytic Application— ***Chamath Vindula Bandara Basnayake***, *Shohreh Hemmati*
4:15 Paper 206e: Designer Hybrid Colloids: A Study of Gold Adsorption Onto Polystyrene to Control Morphologies of Reactive Nanoparticles — ***Joanna Schneider***, *Victoria E. Lee, Jason Liu, Sujit Datta, Rodney Priestley*
4:30 Paper 206f: Rheoelectric Characterization of Oxidized Carbon Nanoparticles As Slurry Active Materials — ***Paolo Ramos***, *Connor Call, Lauren Simitz, Jeffrey Richards*
4:45 Paper 206g: Utilizing Atomic Layer Deposition to Influence Selectivity for Ni Reverse Water Gas Shift Catalysts — ***Megan English***, *Kent J. Warren, Alan Weimer*
5:00 Paper 206h: Targeted Delivery of Surfactants Via Directed Assembly of Nanoparticles at Liquid-Liquid Interfaces By Fine-Tuning Molecular Interactions— ***Mohamed Amen Hammami***, *Genggeng Qi, Bashayer S. Aldakkan, Mazen Kanj, Emmanuel P. Giannelis*

(207) NSF Workshop II: Proposal Writing and Discussions with Program Managers

Monday, Nov 15, 12:30 PM
Virtual, Education Division (04)

Ram Gupta, Chair
Carole Read, Co-Chair

Sponsored by: Career Guidance Committee Liaison

12:30 Paper 207a: Proposal Writing Tutorial — ***Dimitrios Papavassiliou***
1:30 Paper 207b: Interactive Breakout Panels — ***Tim Patten***, *Robert McCabe, Christina Payne, Shahab Shojaei-Zadeh, Steven Zehnder, Mamadou Diallo, Carole Read*

(209) Perovskites, spinels, energy conversion, modeling of these systems

Monday, Nov 8, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 306

Alan Weimer, Chair
Gyeong S. Hwang, Co-Chair

Sponsored by: Material Interfaces as Energy Solutions

3:30 Paper 209a: First-Principles Understanding and Design of Metal Oxides for Photocatalytic Water Splitting — ***Gyeong S. Hwang***
3:51 Paper 209b: Structural and Stability Trends in Single (ABO_3) Perovskite Oxides from DFT-Optimized Bond Valence Structures — *Zachary Bare,* ***Ryan Morelock***, *Christopher Sutton, Charles B. Musgrave*
4:12 Paper 209c: Extracting the RedOx Thermodynamics of Perovskites via Combined Experiment and Theory — *Steven Wilson, Ellen Stechel,* ***Christopher L. Muhich***
4:33 Paper 209d: Materials Discovery and Development for Lower Temperature and Near Isothermal Thermochemical H2 Production — ***Jonathan Scheffe***, *Dylan McCord, Juan C. Nino, Elizabeth Gager, Simon Phillpot, Ximeng Wang*
4:54 Paper 209e: Thermodynamic Characterization of Doped Spinels for Thermochemical Fuel Production — ***Kent J. Warren***, *Justin Tran, Alan Weimer*
5:15 Paper 209f: Sustainable High-Purity Nitrogen Production Via a Coupled PSA-Thermochemical Process for the Ammonia Industry — ***Lena Klaas***, *Dorottya Kriechbaumer, Mathias Pein, Martin Roeb, Christos Agrafiotis, Christian Sattler*
5:36 Paper 209g: High-Purity Nitrogen Production from Air By Pressure Swing Adsorption Combined with $SrFeO_3$ Redox Chemical Looping for Trace Oxygen Removal — ***Brendan Bulfin***, ***Aldo Steinfeld***

(210) Point-of-Need Sensor Applications

Monday, Nov 8, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 200

Ariel Furst, Chair
Yi Zhang, Co-Chair
Evan Wujcik, Co-Chair

Sponsored by: Sensors

3:30 Paper 210a: Invited Talk: Taking Electrochemical Biomolecular Sensors from the Bench to the Clinic — ***Shana Kelley***
3:55 Paper 210b: Sensitive Electrochemical Detection of Pathogenic *E. coli*— ***Ariel Furst***
4:12 Paper 210c: Synthetic Biology Mediated Electrochemical Sensing Strategy— ***Yifan Dai***, *Wei Xu, Rodrigo A Somoza, Jean F. Welter, Arnold I. Caplan, Chung-Chiun Liu*
4:29 Paper 210d: Hydrogel-Encapsulated Gold Nanoshells Prepared By Inverse Emulsion Polymerization As a Biosensor for Sjögren's Syndrome Protein Markers — ***Andrew Murphy***, *Nicholas Peppas*
4:46: Break
5:03 Paper 210f: Silk-Based Microneedle Biosensor for Sustainable Food Supply Chain — ***Doyoon Kim***, *Yunteng Cao, Benedetto Marelli*
5:20 Paper 210h: Engineered CRISPR-Enhance System for Clinical Detection of Sars-COV-2 RNA — *Long Nguyen, Santosh Rananaware, Brianna L. M. Pizzano, Brandon Stone,* ***Piyush Jain***
5:28 Paper 210i: Computational Design of MOF-Based Electronic Noses for Disease Detection By Breath — ***Brian A. Day***, *Christopher E. Wilmer*
5:36 Paper 210j: Interaction of Acetylcholinesterase with Phorate — ***Shalini Shikha***, *Sudip Pattanayek*
5:44 Paper 210k: Hyperspectral Imaging Sensors Enhance on-Line Food Quality and Authenticity Inspection. — ***William Rock***, *Alon Vaisman*
5:52 Paper 210l: Collagen Type II Quantification with Pd@Pt Nanoparticle-Linked Immunosorbent Assay — ***Eunice Kwon***, *Haneen Abusharkh, Bernard Van Wie*

(211) Process Research for Improved Throughput & Efficiency, and Reduced Cost

Monday, Nov 8, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 300

Robert Nunley, Chair
Xue (Ida) Chen, Co-Chair
Mrunmayi Kumbhalkar, Co-Chair

Sponsored by: Process Research and Innovation

3:30 Paper 211a: Modeling and Comprehensive Analysis for an Industrial Complex Coupling Allam Power Cycle, Air Separation Unit, and Ammonia Manufacturing Process — ***Song Wang***, ***Qiang Xu***
4:00 Paper 211b: Application of Mathematical Algorithms for Real Time Optimization of Continuous Flow Extraction Processes — *Eric Gauthier,* ***Boubacar Diallo***
4:30 Paper 211c: Advanced Operating Strategies to Enhance the Performance of Chemical Looping Natural Gas Reforming Processes — ***Fanhe Kong***, *Mandar Kathe, Andrew Tong, L.-S. Fan*
5:00 Paper 211e: Data-Driven Predictive Model and Optimization Based on Machine Learning on Steam Reforming Process — ***Jaewon Lee***, *Seokyoung Hong, Youngjin Kim, Hyungtae Cho, Myungjun Kim, Hyungjoon Yoon, Junghwan Kim, Il Moon*

(212) Prof C A Floudas: Five Years later – Where are we now?

Monday, Nov 8, 3:30 PM
Sheraton Back Bay, Independence Ballroom West

Chrysanthos Gounaris, Co-Chair
George A. Khoury, Co-Chair

Sponsored by: Systems and Process Operations

3:30 Paper 212e: Impact of Chris Floudas on Recent Developments in Process Synthesis and Flexibility Analysis — ***Ignacio Grossmann***
3:49 Paper 212a: The Automated NSF Panel Generator: An Elegant Optimal Solution to a Multi-Resource and Preference-Constrained Generalized Assignment Problem — ***Triantafillos Mountziaris***
4:08 Paper 212g: The Phase Behavior of Supercooled Water: Recent Computational Results — ***Pablo Debenedetti***
4:27 Paper 212b: Manifold Learning for Accelerating Coarse-Grained Optimization — ***Ioannis G. Kevrekidis***
4:46 Paper 212c: Optimization Frameworks As Discovery Tools in Metabolic Networks and Protein Design — ***Costas D. Maranas***
5:05 Paper 212f: Multi-Objective Optimisation for Mixed-Integer Nonlinear Optimization Problems: Algorithms and Applications to Molecular Modelling and Design — *Ye Seol Lee, Edward Graham, Amparo Galindo, George Jackson,* ***Claire Adjiman***
5:24 Paper 212d: Data-Based Process Systems Methods and Applications— ***Marianthi Ierapetritou***

5:43 Paper 212h: Energy Price Index Framework and Tools – Five Years Later— *Stefanos Baratsas, **Efstratios N. Pistikopoulos***

(213) Student Support and Professional Skill Development

Monday, Nov 8, 3:30 PM
Sheraton Back Bay, Republic Ballroom A

Jennifer Pascal, Chair
Sarah Wilson, Co-Chair
Charles Coronella, Co-Chair

Sponsored by: Education

3:30 Paper 213a: Professional Skill and Attribute Instruction in a Capstone Design Course at an Hispanic-Serving Institution — ***Matthew Alexander***
3:48 Paper 213b: Holistic, Wrap-Around, Advising Model to Support Student Success and Professional Development — ***Julie Hasenwinkel**, Sarah Mack*
4:06 Paper 213c: "10.801: Project Management and Problem Solving in Academia and Industry" — a New Course for MIT Graduate Students in Chemical Engineering Practice — ***Robert T. Hanlon**, Kai-Jher Tan, **Zongyu Gu**, T Alan Hatton*
4:24 Paper 213d: Relationship between Students' Engineering Identity and Self-Efficacy and Participation in an Engineering Education Enrichment Program— ***Hengameh Bayat**, Catherine Brewer, Sandra Way*
4:42: Break
5:00 Paper 213f: Student-Driven Career-Focused Development of Design Engineering Skills — ***Jason White**, John Davis, Evren Bicakci, Haruka Shudo, Mason Lydon, Samuel Clark*
5:18 Paper 213g: The Prevalence of Imposter Phenomenon in Undergraduate and Graduate Chemical Engineers — ***Sarah Wilson**, Ellen Usher, Natalie Ban, Isabella Armstrong*

(214) The Hard Skills of Emotional Intelligence for Effective Engineering Leaders

Thursday, Nov 18, 8:00 AM
Virtual, Management Division (05)

Gayle Gibson, Chair

Sponsored by: Management Division

8:00 Paper 214a: The Hard Skills of Emotional Intelligence for Effective Engineering Leaders — ***Gayle Gibson**, **David Caruso***

(215) Thermodynamic and Transport Properties Under Pressure

Monday, Nov 8, 3:30 PM
Sheraton Back Bay, Back Bay Ballroom A

Sabine Enders, Chair
Steven Saunders, Co-Chair

Sponsored by: High Pressure

3:30 Paper 215a: Thermal Transitions and Physical Foaming of an Ethylene/Acrylic Acid/n-Butyl Acrylate Ionomer with Carbon Dioxide — *Joseph Sarver, Joshua Rasco, Xian Jiang, Jozef Van Dun, **Erdogan Kiran***
3:49: Break
4:07 Paper 215c: Transport Properties of Imidazolium Ionic Liquids Saturated with Compressed Gases — ***Aaron Scurto**, **Karim Al-Barghouti***
4:26 Paper 215d: Fast and Robust Three-Phase Free-Water Flash Calculations— ***Dan Vladimir Nichita***
4:45 Paper 215e: High Pressure Thermodynamics and Viscosity of Group IV Base Oil Lubricants Modified with Polyisobutylene Dispersants and Their Modeling with Free Volume and Density-Scaling — ***Katrina Avery**, Mackenzie Roach, Joseph Sarver, Erdogan Kiran, Mark Devlin*
5:04: Break
5:22 Paper 215g: Supercritical CO_2 extraction of Resin and Rubber from Guayule (*Parthenium argentatum* A.Gray) Biomass — ***Mostafa Dehghanizadeh**, Catherine Brewer*
5:40 Paper 215h: Confined Batch Foaming of Rubbery Elastomers with Carbon Dioxide Using a Mold — ***Joseph Sarver**, Jenna Sumey, Richard Whitfield, Erdogan Kiran*

(217) Waste Plastic - Recycle, Reuse and Remediation Strategies

Monday, Nov 8, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 309

Jeffrey Seay, Chair
Amy E. Landis, Co-Chair
Robert Peters, Co-Chair

Sponsored by: Solid and Hazardous Waste

3:30 Paper 217a: Thermochemical Co-Conversion of Waste Polyolefins with Low-Rank Aromatic-Rich Hydrocarbons into an Intermediate of High-Quality Anisotropic Pitch — ***Wenjia Wang**, Ignacio Preciado, Eric Eddings*
3:45 Paper 217b: Global Issues in Plastic Waste: Community Focused Management Approaches — ***Shelby Browning**, Jeffrey Seay, Robert Peters*
4:00 Paper 217c: A Material Flow Analysis for Sustainable End-of-Life Plastic Management — ***John Chea**, Kirti Yenkie, Joseph Stanzione III, Gerardo Ruiz-Mercado*
4:15 Paper 217d: Use of Surfactants to Deink Plastics — *Asmita Baruah, **Brian Grady***
4:30 Paper 217e: Study of the Viscosity and Thermal Characteristics of Polyolefins / Solvent Mixtures: Applications for Plastic Pyrolysis — ***Ali Zolghadr**, Azarnoosh Foroozandehfar, Daniel Kulas, David Shonnard*
4:45 Paper 217f: Waste Plastics and Microplastics in Africa: Negative Impacts and Opportunities — *Gaber Abdellatif, **Mohamed Mostafa**, Ahmed S. Mahmoud, **Robert Peters***

(218) Water Reuse and Recycling

Monday, Nov 8, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 308

Kirti Yenkie, Chair
Toufiq Reza, Co-Chair
Deepak Sharma, Co-Chair

Sponsored by: Water

3:30 Paper 218a: Equipment and Method for Batch Screening of Methanotroph-Microalgae Cocultures for Waste-to-Value Conversion — ***Loyal Murphy**, Kiumars Badr, William Whelan, Q. Peter He, Jin Wang*
3:55 Paper 218b: Sustainability and Economic Evaluation of Tannery Wastewater Treatment Pathways Using the P-Graph Approach — ***Emmanuel A Aboagye**, Maya Desai, Carley Tran, Jean Pimentel, Akos Orosz, Heriberto Cabezas, Ferenc Friedler, Kirti Yenkie*
4:20 Paper 218c: Modeling, Simulation and Optimization of a Synergistically Mixed Blowdown Water and Produced Water Wastewater Treatment Process— ***Hunter Barber**, Fernando V. Lima*
4:45 Paper 218d: Effluent Reduction in Pulp and Paper Manufacturing: Paper Machine White Water Recycle in Bleaching Section — ***Amod Parkhi**, Selen Cremaschi, Zhihua Jiang*
5:10 Paper 218e: Evaluation of Dioxins and Their Precursors in Fly Ashes and Wastewater Generated in the WET Scrubbing of Flue Gases from Sugarcane Bagasse Boilers — ***Murilo Innocentini**, Pedro Pires, Cristina Paschoalato, **Tapas K. Das***
5:35 Paper 218f: Assessing Ozonation Suitability for Secondary Effluent Treatment Via Virtual Piloting with the Amozone Model — ***Giacomo Bellandi**, Roberta Muoio, Miguel Daza, Usman Rehman, Ingmar Nopens, Stefan Weijers, Peter van Dijk, Ruud Schemen, Tom Weijtmans, **Wim Audenaert***

(219) MAC Eminent Engineers Awards Poster Session

Monday, Nov 8, 5:30 PM
John B. Hynes Veterans Memorial Convention Center, 203

Kazeem Olanrewaju, Chair

Sponsored by: Minority Affairs Committee (MAC)

Poster 219a: MAC Poster #1
Poster 219b: Bioconversion of plastic wastes into value-added products using thermal oxo-degradation — ***Efrain Rodriguez-Ocasio***
Poster 219c: Kasim A. Adewuyi Poster — ***Kasim Adewuyi***
Poster 219d: Impact of Crowding Agent on Supramolecular Complexation— ***Busayo Alagbe***
Poster 219e: Thermal Properties of Heat-treated Coal Under Inert Conditions— ***Chiderah Chukwuka***
Poster 219f: Suraj Aryan Poster — ***Suraj Aryan***
Poster 219g: Preliminary risk assessment of traffic accidents in Colombia involving loss of containment of liquid hydrocarbons — ***Natalia Godoy Silva***
Poster 219h: Hierarchical Zeolite Composite Catalyst from the Aerosol-assisted Encapsulation of ZSM-5in Ordered MCM-41 Microspheres — ***Azeem Farinmade***
Poster 219i: Metabolic Modeling of *Pseudomonas Putida* KT2440 to Understand and Improve the Breakdown of Plastic Waste — ***Leah Lewis***
Poster 219j: Biogas Production By Co-Digestion of Goat Manure with Two Crop Residues
Poster 219k: The Pathophysiological Effects of Fluid-Structure Interaction of Species Transported and Transformed from Ambient to Human Respiratory System — ***Unyime Effiong***
Poster 219l: Roneisha Blakeney
Poster 219m: Bianca Mitchell — ***Bianca Mitchell***
Poster 219n: MAC Poster #14
Poster 219o: MAC Poster #15
Poster 219p: MAC Poster #16

(221) MAC Eminent Engineers Awards Ceremony

Monday, Nov 8, 6:00 PM
John B. Hynes Veterans Memorial Convention Center, 203

Sponsored by: Minority Affairs Committee (MAC)

(222) 2020 Hoover Medal Lecture

Monday, Nov 8, 6:15 PM
John B. Hynes Veterans Memorial Convention Center, Ballroom B

John Anderson, Chair

Sponsored by: Awards Committee

6:15: Introductory Remarks
6:25 Paper 222a: Reclaiming the Engineering in the Minds of the Public:The Unheralded, Underappreciated, and Misunderstood Method that Built Our Modern World — ***William Hammack***

(223) SBE's James E. Bailey Award Lecture

Tuesday, Nov 9, 7:00 PM
John B. Hynes Veterans Memorial Convention Center, 302

Sponsored by: Awards Committee

7:00: Presentation of Biotechnology Progress Award for Excellence in Biological Engineering Publication
7:05 Paper 223a: Synthetic Biology: Life Redesigned — ***James J. Collins***

(224) 3D Printing of Functional Materials

Tuesday, Nov 9, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 202

Arit Das, Chair

Bradley Sutliff, Co-Chair

Sponsored by: 3D Printing

8:00 Paper 224a: Guest Speaker
8:35: Break
8:58 Paper 224c: Personalizing Wound Dressings Via 3D Printing for the Treatment of Thermal Burns — ***Jia Heng Teoh***, *Anbu Mozhi, Chi-Hwa Wang*
9:21 Paper 224d: 3D Printing of Pharmaceuticals-Exploring Process Parameters and Structure Dry Weight Relations — ***Mohammad Azad***, *Georgia Kimbell, Deborah Olawuni*
9:44 Paper 224e: Novel Polyester-Based Thermoplastic Elastomers for 3D-Printed Personalised Urethra Pessaries — ***Martin Spörk***, *Florian Arbeiter, Ioannis Koutsamanis, Hrvoje Cajner, Matthias Katschnig, Simone Eder*
10:07 Paper 224f: 3D Printing of Chiral Liquid Crystal Elastomers Using Cellulose Nanocrystals — ***Mohsen Esmaeili***, *Kyle George, Nader Taheri-Qazvini, Monirosadat Sadati*

(225) Advances in Antimicrobial and Antifouling Materials

Tuesday, Nov 9, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 310

Caitlin Howell, Co-Chair
Connie Chang, Co-Chair

Sponsored by: Microbes at Biomedical Interfaces

8:00 Paper 225a: Antimicrobial Surface Coatings to Reduce COVID-19 Spread— ***Zachary Whitermore***, *Dorin V. Preda, Peter A. Warren, Min Song, Cameron R. McConnell, Alex W. Moerlein, Nathan R. Shipley, John H. Connor, Scott Seitz*
8:30 Paper 225b: Chemorepellent-Loaded Polymeric Nanocarriers for Biofilm Inhibition — ***Tracy Kuper***, *Leon Z. Wang, Sujit Datta, Robert K. Prud'homme, Roseanne M. Ford*
9:00 Paper 225c: Semi-Synthetic Outer Membrane Vesicles for Controlled Antibiotic Delivery — *Shannon Collins, Daniel Sahlman,* ***Angela Brown***
9:30 Paper 225e: Self-Locomotive Antimicrobial Microparticles for Enhanced Biofilm Removal — ***Yu-Heng Deng***, *Tomas Ricciardulli, Jungeun Won, Stephen Boppart, David Flaherty, Hyunjoon Kong*
10:00 Paper 225d: Antibiofilm Activity of Enzyme and pH Responsive Layered Gelatin Nanoparticles — ***Yingying Wang***, *Anita Shukla*

(226) Advances in Computational Methods and Numerical Analysis I

Tuesday, Nov 9, 8:00 AM
Sheraton Back Bay, Independence Ballroom East

Ali Mesbah, Chair
Satyajith Amaran, Co-Chair

Sponsored by: Applied Mathematics and Numerical Analysis

8:00 Paper 226a: Learning Partial Differential Equations in Emergent Coordinates — *Felix Kemeth, Thomas Bertalan, Thomas Thiem,* ***Ioannis G. Kevrekidis***
8:19 Paper 226b: Computer Modeling of Aerosol Particle Transport through Lung Mucosa — ***Blake Bartlett***, *Yu Feng, Catherine Fromen,* ***Ashlee Ford Versypt***
8:38 Paper 226c: A Closed Loop Control Perspective on the Reconfiguration of Brain Networks — ***Ilias Mitrai***, *Catherine Stamoulis, Prodromos Daoutidis*
8:57 Paper 226d: Tractable Global Solutions to Chance-Constrained Bayesian Optimal Experiment Design for Arbitrary Prior and Noise Distributions — ***Diogo Rodrigues***, *Georgios Makrygiorgos, Ali Mesbah*
9:16 Paper 226f: Physics-Informed Neural Network for Solving 2-D Heat Transfer Problems without Labeled Data — ***Zhibin Lu***, *Mingjian Li, Zengrong Su, Chang He, Bingjian Zhang, Qinglin Chen*
9:35 Paper 226g: Investigating the Spatiotemporal Patterns of Bacteria Using Computational Tools — ***Kimberly Bowal***
9:54 Paper 226h: Integrated Computational and Experimental Study to Dissect the Stress Response of Maize Root — ***Niaz Chowdhury***, *Wheaton Schroeder, Dongdong Zhang, Margaret N. Simons, Bertrand Hirel, Edgar Cahoon, Costas D. Maranas, Rajib Saha*
10:13 Paper 226e: Optimal Artificial Neural Network Architecture Synthesis and Input Selection — *Erdal Aydin,* ***Hasan Sildir***

(227) Advances in global optimization

Tuesday, Nov 9, 8:00 AM
Sheraton Back Bay, Independence Ballroom West

Kamil Khan, Co-Chair
Radhakrishna Tumbalam Gooty, Co-Chair

Sponsored by: Systems and Process Operations

8:00 Paper 227a: Alternative Regularization Schemes in Outer-Approximation Algorithms for Convex MINLP — ***David E. Bernal***, *Zedong Peng, Jan Kronqvist, Ignacio Grossmann*
8:19 Paper 227b: Guaranteed Accuracy of Machine Learning-Based Surrogate Models Using Bilevel Optimization — ***Danimir T. Doncevic***, *Artur Schweidtmann, Tim Kerkenhoff, Manuel Dahmen, Alexander Mitsos*
8:38 Paper 227c: Computing Lower Bounds in Global Optimization By Tractably Sampling Convex Relaxations — *Yingkai Song, Huiyi Cao,* ***Kamil Khan***
8:57 Paper 227d: An Improved Implementation of the Rpd Method for Computing Convex Relaxations for Global Dynamic Optimization — ***Jason Ye***, *Joseph K. Scott*
9:16 Paper 227e: Approaches to Improve Bilinear Relaxations in Reduced-Space — ***Matthew Wilhelm***, *Matthew Stuber*
9:35 Paper 227f: Tightening Constraints for Bilinear Terms with Semi-Continuous Variable and Nontrivial Bounds — ***Yifu Chen***, *Christos Maravelias*
9:54 Paper 227g: Formulations and Restrictions for the Pooling and Multiperiod Pooling Problems — ***Calvin Tsay***, *Francesco Ceccon, Ruth Misener*
10:13 Paper 227h: Global Optimization for Clustering Problems with 200,000 Samples — ***Mingfei Shi***, *Kaixun Hua, Yankai Cao*

(228) Advances in Metabolic Engineering- Eukaryotic Organisms

Tuesday, Nov 9, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 111

Sijin Li, Chair
Aditya Kunjapur, Co-Chair

Sponsored by: Bioengineering

8:00 Paper 228a: A Repackaged CRISPR/Cas9 Platform Recasts Non-Homologous End Joining As a Beneficial Instrument in Nonconventional Yeast Engineering — ***Deon Ploessl***, *Zengyi Shao*
8:18 Paper 228b: Engineering a Global Regulatory System Potentiates Rapid Growth of *Saccharomyces Cerevisiae* on Numerous Non-Native Substrates— ***Sean Sullivan***, *Vikas Trivedi, Venkatesh Endalur Gopinarayan*
8:36 Paper 228c: Partnering Anaerobic Fungi and Engineered *KluyveromycesMarxianus* Enables Direct and Efficient Production of Fragrances and Fuels from Agricultural Residues — *Ethan Hillman, Mengwan Li, Casey Hooker, Jacob A. Englaender, Ian Wheeldon,* ***Kevin Solomon***
8:54 Paper 228d: Title: Metabolic Engineering of the Non-Conventional Yeast, *Kluyveromyces Marxianus*, for Enhanced Biosynthesis of a Platform Biochemical— ***Danielle Bever-Sneary***, *Nancy Da Silva*
9:12 Paper 228e: Exploration of Epigenetic Regulation and Development of Global and Targeted Epigenetic Engineering Tools for *Taxus* Plant Cell Culture— ***Cassandra Brzycki Newton***, *Sangram Lenka, Gabrielle Mazzoni, Emily Whittles, Michaela Gamache, Eric Young, Susan Roberts*
9:30 Paper 228f: Reaction Compartmentalization Leads to Enhanced Production of PHA in *Yarrowia Lipolytica* — ***Michael Spagnuolo***, *Meredith Bailey, Mark Blenner*
9:48 Paper 228g: *Unlocking the Biotech Potential of Anaerobic Gut Fungi*— ***Michelle O'Malley***

(229) Advances in Zeolite Science and Technology II - Applications and Explorations in New Catalysis (Invited Talks)

Tuesday, Nov 9, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 208

Aditya Bhan, Chair
Robert Saxton, Co-Chair

Sponsored by: Advances in Zeolite Science and Technology

8:00 Paper 229c: Subnanometric Metal Clusters and Single Metal Atoms inside Zeolites — ***Pedro Serna Merino***, *Manuel Moliner, Avelino Corma, Aida Rodriguez-Fernandez, Sara Yacob, Chris Kliewer*
8:25 Paper 229d: Transport in Small-Pore Zeolites — ***Peter Ravikovitch***
8:50 Paper 229f: Adsorption of Carbon Dioxide with Small Pore, Cage Containing Zeolites — ***Donglong Fu***, *Youngkyu Park, Faisal Alshafei, Mark Davis*
9:15: Break
9:25 Paper 289a: Confinement and Diffusion Effects in Hierarchical Zeolites for Diverse Reaction Networks — *Hayat Adawi,* ***Michele Sarazen***
9:50 Paper 289f: Resolving Impacts of Acidity and Morphology on the Decarboxylation of γ-Valerolactone — ***Jesse Bond***, *Xinlei Huang*
10:10 Paper 289g: Unique Roles of Heteroatoms in the Synthesis of Zeolite Catalysts — ***Deependra Parmar***, *Adam Mallette, Lars Grabow, Jeffrey Rimer*

(230) Allies and Advocates Training

Tuesday, Nov 9, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 204

Audie Thompson, Chair
Carlos M Rinaldi-Ramos, Co-Chair

Sponsored by: Topical Conference: The Role of Intersectionality in Chemical Engineering

(231) Amorphous and Crystalline Particle Engineering in Pharmaceuticals and Other Novel Materials

Tuesday, Nov 9, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 302

Lotfi Derdour, Chair
Mo Jiang, Co-Chair
Ryan Snyder, Co-Chair

Sponsored by: Crystallization and Evaporation

8:00: Welcoming Remarks
8:03 Paper 231a: Design and Use of a Thermogelling Methylcellulose Nanoemulsion to Formulate Nanocrystalline Oral Dosage Forms — ***Liang-Hsun Chen***, *Patrick S. Doyle*
8:24 Paper 231b: Particle Formation from the Drying of Liquid Droplets Containing Insoluble Material — ***Siavash Zamani***, *Aaron Morris*
8:45 Paper 231c: Development of Apap Tablets in a 3D Mold Using Drops of Dissolved Excipients — ***Sheena Reeves***, *Nigel Brooks Jr., Yazmine Rincon*
9:06 Paper 231d: Wet Milling with in-Line Fines Dissolution — ***Paria Coliaie***, *Moussa Boukerche, John G. Gaertner, Daniel Pohlman, Manish Kelkar, Meenesh Singh, Nandkishor K. Nere*
9:27 Paper 231e: Autocatalytic Initiation Followed By Oriented Attachment Governs the Nucleation and Crystal

Growth of MOF Crystals — ***Anish Dighe***, *Luke Huelsenbeck, Prince Verma, Kevin Stone, Meenesh Singh, Gaurav Giri*
9:48 Paper 231f: 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*
10:09 Paper 231g: Thermodynamic Modeling of Competing Crystal Species from a MIL-53 Metal Organic Framework (MOF) Reaction — ***Andrew Garcia***, *Dirk Steyn III, Sergey Vasenkov, Kirk J. Ziegler*

(232) Area Plenary: Bionanotechnology (Invited Talks)

Tuesday, Nov 9, 8:00 AM
Marriott Copley Place, Simmons

Lorraine Leon, Chair
Elizabeth Nance, Co-Chair
Catherine Fromen, Co-Chair

Sponsored by: Bionanotechnology

8:00 Paper 232a: Cellular Hitchhiking for Targeting Nanoparticles — ***Samir Mitragotri***
8:50 Paper 232b: Nanomedicine for Improved Ocular Drug Delivery — ***Laura Ensign***
9:40 Paper 232c: Nanoparticle Physiochemical Design Features to Modulate Pulmonary Innate Immune Cell Response — ***Catherine Fromen***

(233) Area Plenary: Interfacial Phenomena (Invited Talks)

Tuesday, Nov 9, 8:00 AM
Sheraton Back Bay, Back Bay Ballroom A

Marina Tsianou, Chair
Christopher Wirth, Co-Chair

Sponsored by: Interfacial Phenomena

(234) Biomanufacturing with Advanced Mammalian Cell Culture Technologies

Tuesday, Nov 9, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 110

Amir Sheikhi, Chair
Amol Janorkar, Co-Chair

Sponsored by: Bioengineering

8:00 Paper 234a: Metabolite Monitoring of Mesenchymal Stromal Cell Cultures By Spontaneous Raman Spectroscopy — ***Nili Persits***, *Camille Farruggio, Krystyn Van Vliet, Rajeev J. Ram*
8:21 Paper 234b: Shield: A Platform for Fast and Simple Screening of Anti-Silencing DNA Elements in Human Cells — ***Meng Zhang***, *Srija Matukumalli, Huimin Zhao*
8:42 Paper 234c: Predictive *in silico* Models for Cell Culture Process Development for Biologics Manufacturing — ***Aparajita Dasgupta***, *Jackie Gonzalez, Michael Chin, Andrew Fiordalis, Lijuan Li, Nan Wang, Shan Tie, John Love, Connor Coley*
9:03 Paper 234d: Shear Stress Effects on Energy Metabolism and Exosome Secretion of Human Mesenchymal Stem Cells in a Novel Pbs Vertical Wheel Bioreactor — ***Richard Jeske***, *Xuegang Yuan, David Meckes, Sunghoon Jung, Yan Li*
9:24 Paper 234e: Modeling the Effect of pH on Chinese Hamster Ovary Cell Metabolism and Glycosylation to Optimize the Production of Monoclonal Antibodies — ***Jayanth Venkatarama Reddy***, *Ashwin Dravid, Eleftherios Papoutsakis, Marianthi Ierapetritou*
9:45 Paper 234f: A Metaheuristic Investigation of the Impact of Nutrient Supplementation Strategies on the Growth and Productivity of Mammalian Cell Cultures — ***Ricardo Suarez Heredia***, *Nishanthi Gangadharan, Alexandros Kiparissides, Duygu Dikicioglu*
10:06 Paper 234g: Looking inside and out: Addressing Bioprocessing Challenges in the Biopharma Industry — ***Michael Betenbaugh***

(235) Biomimetic Materials I

Tuesday, Nov 9, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 209

R. Helen Zha, Chair
Xi Chen, Co-Chair
Handan Acar, Co-Chair
Nader Taheri-Qazvini, Co-Chair

Sponsored by: Biomaterials

8:00 Paper 235a: Protein Based Biomimetic Materials — ***Melik Demirel***
8:36 Paper 235b: Greasing Proteins Wheels: Genetically Encoded Amphiphiles with Programmable Architecture and Assembly — ***Davoud Mozhdehi***
8:54 Paper 235c: Hybrid Protein-DNA and Peptide-DNA Nanostructures— ***Nicholas Stephanopoulos***
9:12 Paper 235d: Water-Responsive Actuation of *Bombyx Mori* silk/Silica Nanocomposites — ***Yeojin Jung***, *Samaneh Sharifi Golru, Tai-De Li, Elizabeth Biddinger, Raymond S. Tu, Xi Chen*
9:30 Paper 235e: Peptide Stereocomplexes As Dynamic Elements of Biomaterials — *Israt Jahan Duti, Connor Amelung, Jonathan Florian, Vincent Gray, Emma Laudermilch, Kyle Lampe,* ***Rachel Letteri***
9:48 Paper 235f: Engineering Peptides for an All-Inclusive Immune Response— *Gokhan Gunay, Seren Hamsici,* ***Handan Acar***
10:06 Paper 235g: Tunable Molecular Self-Assembly of Dynamic Oligopeptide Materials — ***Matthew Webber***

(236) Carbon Nanomaterials: Dispersion, Surface Structure, and Biointeractions

Tuesday, Nov 9, 8:00 AM
Marriott Copley Place, Wellesley

Anju Gupta, Chair
Jung-Sheng Wu, Co-Chair
Gözde Demirer, Co-Chair

Sponsored by: Carbon Nanomaterials

8:00: Break
8:25 Paper 236b: Thermomechanical Properties of Nanodiamond Superstructures in Interlayer-Bonded Twisted Bilayer Graphene — *Mengxi Chen, Asanka Weerasinghe, Andre R. Muniz, Afnan Mostafa, Ashwin Ramasubramaniam,* ***Dimitrios Maroudas***
8:50 Paper 236c: Interactions of Graphene Oxide Nanosheets with Blood-Related Entities and Their Implications for Hematological Disorders — ***Kenry .***
9:15: Break
9:40 Paper 236e: Sustainable Production of Graphene from Petroleum Coke Using Electrochemical Exfoliation — ***Micah Green***, *Rohan Hule, Sergey Yakovlev, Sundararajan Uppili*
10:05 Paper 236f: Interleukin 6 (IL-6) Targeted Corona Phase Molecular Recognition Using Fluorescent Nanosensors — ***Xiaojia Jin***, *Michael A. Lee, Xun Gong, Naveed Bakh, Michael S. Strano*

(238) Clinical Impacts of Micro- and Nano-Scale Technologies

Tuesday, Nov 9, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 109

Gulden Camci-Unal, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

8:00 Paper 238a: Identification of Carbonyl Compounds in Exhaled Breath Using UHPLC-MS — ***Zhenzhen Xie***, *Xiao-an Fu, James Morris*
8:18 Paper 238b: A Scalable Gold Nanoparticle-Templating Method for Generating Erodible Drug Microparticles without Use of Exogenous Biodegradable Polymers — *Hanieh Safari,* ***Michael Felder***, *Omolola Eniola-Adefeso*
8:36 Paper 238c: The Mechanical Impact of Rigid Red Blood Cells in Sickle Cell Disease on Leukocyte Adhesion Performance in Blood Flow — *Mario Gutierrez, Omolola Eniola-Adefeso, Mark Shamoun,* ***Logan Piegols***
8:54 Paper 238d: Ultrasensitive Single-Molecule Detection of a Retrotransposon-Encoded Protein As a Multi-Cancer Blood Biomarker— ***Connie Wu***, *Limor Cohen, Martin Taylor, Yasmeen Senussi, David Ting, David Walt, Kathleen Burns*
9:12 Paper 238e: Polymeric Drug Carriers Modulate Platelet Adhesion in Thromboinflammation — ***Alison Banka***, *Lola Eniola-Adefeso*
9:30 Paper 238h: Unconventional Biomaterials to Improve Human Health— ***Gulden Camci-Unal***
9:48 Paper 238g: A Click Chemistry Amplified Nanopore (CAN) Assay for Ultrasensitive Quantification of Infectious Diseases Related Biomarkers in Clinical Samples (Invited Speaker) — ***Chang Liu***

(239) Colloidal Hydrodynamics

Tuesday, Nov 9, 8:00 AM
Sheraton Back Bay, Constitution A

Christian Aponte-Rivera, Chair
Joseph Barakat, Co-Chair

Sponsored by: Fluid Mechanics

8:00 Paper 239a: Jamming Distance Governs the Viscoelasticity and Shear Thickening of Rough Colloids — *Shravan Pradeep, Mohammad Nabizadeh, Alan Wessel, Alan Ranjit Jacob, Safa Jamali,* ***Lilian Hsiao***
8:15 Paper 239b: Dynamics of Semiflexible Colloidal Sheets in Shear Flow: Thermal Fluctuations — ***Kevin Silmore***, *Michael S. Strano, James Swan*
8:30 Paper 239c: Bilayer Aggregate Microstructure Determines Viscoelasticity of Lung Surfactant Suspensions — ***Clara Ciutara***, *Joseph Zasadzinski*
8:45 Paper 239d: Dynamics and Rheology Characterization of Solvent Segregation Driven Gel (SeedGel) — ***Yuyin Xi***, *Ryan P. Murphy, Yun Liu*
9:00 Paper 239e: The Role of Hydrodynamic Interactions on the Aggregation Kinetics of Sedimenting Colloidal Particles — ***Lorenzo Turetta***, *Marco Lattuada*
9:15 Paper 239f: Vitrification Is a Spontaneous Non-Equilibrium Transition Driven By Osmotic Pressure — *Jialun Wang,* ***Roseanna Zia***
9:30 Paper 239g: Coupling between Attractions and Repulsions in Flow of Colloidal Suspensions — ***Patrick Underhill***
9:45 Paper 239h: Mobility of Binary Tri-Axial Ellipsoidal Particles — ***Isaac Torres Diaz***

(240) Complex Fluids

Tuesday, Nov 9, 8:00 AM
Sheraton Back Bay, Constitution B

Sujit Datta, Chair
Alexandra V. Bayles, Co-Chair

Sponsored by: Fluid Mechanics

8:00 Paper 240a: Constitutive Modeling of Dilute Wormlike Micelle Solutions: Shear-Induced Structure, Transient Dynamics, and Inhomogeneous Flows— ***Richard Hommel***, *Michael Graham*
8:15 Paper 240b: Effects of Chain Length and Polydispersity on Shear Banding in Simple Shear Flow of Entangled Polymeric Melts — ***Mahdi Boudaghi***, *Brian Edwards, Bamin Khomami*
8:30 Paper 682a: Elastic Turbulence Generates Anomalous Flow Resistance in Porous Media — ***Christopher Browne***, *Sujit Datta*
8:45 Paper 240d: Population Balances for Full-Chain Constitutive Models of Living Polymers — ***Joseph Peterson***, *Michael Cates*
9:00 Paper 240e: Characterization of Inter-Particle Friction in Suspensions Using Enhanced Hydrodynamic

Resistance Approach — ***Madhu Venkata Rama Krishna Majji***, *James Swan*
9:15 Paper 240f: Non-Equilibrium Dynamics of Ring-Linear Polymer Solution Blends: Concentration and Molecular Weight Effects — ***Charles Young***, *Charles Sing*
9:30 Paper 240g: Numerical Simulations of Free-Surface Flows of a Carbopol Solution — ***Josh McConnell***, *Weston Ortiz, Anthony McMaster, Anne Grillet, Rekha R. Rao*
9:45 Paper 240i: Criteria Governing Rod Formation and Growth in Polymer Micelles — *Patrick McCauley, Satish Kumar,* ***Michelle Calabrese***
10:00 Paper 240j: Fingerprinting Complex Fluid Structural Response in Complex Processing Flows — *Patrick T. Corona, Barbara Berke, L. Gary Leal, Marianne Liebi,* ***Matthew Helgeson***

(241) Computing and Data Science in ChE Education

Tuesday, Nov 9, 8:00 AM
Sheraton Back Bay, Republic Ballroom A

Manuela Ayee, Chair
Arthur Hersel, Co-Chair
Jason White, Co-Chair

Sponsored by: Undergraduate Education

8:00 Paper 241a: How to Make a Data Science Curriculum Embrace Engineering Domains and Vice Versa — ***S. Joe Qin***, *Zijun Zhang, Xiang Zhou*
8:18 Paper 241e: Interactive Software for Teaching Multivariable Data Analytics— *Joachim Schaeffer,* ***Richard D. Braatz***
8:36 Paper 241b: Chemical Engineering Students' Perception of and Attitudes Towards Data Science — ***Daisaq Cyrilla***, ***Betul Bilgin***
8:54 Paper 241c: Development of Static and Dynamic Simulation-Based Active-Learning Modules for Chemical Engineering Curriculum — ***Brent Bishop***, *Hunter Barber, Fernando V. Lima, Richard Turton*
9:12 Paper 241d: Introducing Students to Open-Source Partial Differential Equation Solver Codes in Python — ***Pavan Inguva***, *Vijesh Bhute, Pierre Walker, Thomas Cheng*
9:30 Paper 241f: A Two-Fer Scheme: Employing Undergraduates to Develop Programming and Automation Modules for the Undergraduate Curriculum— ***Maureen Tang***, *Cameron F. Abrams, Richard Cairncross, Aviel Chaimovich, Aaron T. Fafarman, Andrea Falcone, Kenneth Lau, Joshua Snyder, Masoud Soroush, John Speidel, Michael J. Walters*
9:48 Paper 241g: Using Templates for Making Programming Languages More User Friendly — ***Mordechai Shacham***, *Neima Brauner, Robert Hesketh, Nicholas Chase, Jordan C. Holman*
10:06 Paper 241h: Matlab Based Applications As Accessible and Interactive Educational Modules to Advance Spectroscopic Understanding — ***Jakub Konkol***, *Justin Marlowe, George Tsilomelekis*

(242) Concentrated Solar Power Generation and Chemical Processing I

Tuesday, Nov 9, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 313

Wojciech Lipinski, Chair
Nick AuYeung, Co-Chair
Christopher L. Muhich, Co-Chair
Ashley Pennington, Co-Chair
Alexandre Yokochi, Co-Chair

Sponsored by: Sustainable Energy

8:00 Paper 242a: Development of low-cost Receivers for Parabolic Trough Assembly for developing countries like India: Optical and Thermal optimization— ***Mihir Panda***, *Ramchandra G. Patil, Sudhir V. Panse, Jyeshtharaj B. Joshi, Vishwanath Dalvi*
8:18 Paper 242b: Solar Thermochemical Water Splitting Using Iron-Aluminate Spinels — ***Kent J. Warren***, *Justin Tran, Scott Rowe, Alan Weimer*
8:36 Paper 242c: Numerical Simulation of Concentrated Solar Energy Absorption in Packed and Fluidized Bed Systems — ***Zeyuan Gao***, *Javad Abbasian, Hamid Arastoopour*
8:54 Paper 242d: Operational Limits of Redox Metal Oxides Performing Thermochemical Water Splitting — ***Alicia Bayon***, *Alberto de la Calle, Ellen Stechel, Christopher L. Muhich*
9:12 Paper 242e: Towards Chemical Equilibrium in Thermochemical Water Splitting — ***Alberto de la Calle***, *Ivan Ermanoski, Ellen Stechel*
9:30 Paper 242f: Kinetic Investigation of Iron Aluminate-Based Materials for Fuel Production — ***Justin Tran***, *Carter Wilson, Kent J. Warren, Alan Weimer*
9:48 Paper 242g: An Optimization-Based Framework for Material Selection and System Design for Integrating Thermochemical Energy Storage in Solar Power Systems — ***Ishan Bajaj***, *Xinyue Peng, Christos Maravelias*
10:06 Paper 242h: Economic Analysis and Environmental Impact of a Novel Solar Parabolic Trough Plant Used for Industrial Process Heat That Utilizes Flexible Heat Integration — ***Jake Immonen***, *Kasra Mohammadi, Kody Powell*

(243) Control Strategies in Pharmaceutical Development and Manufacturing I

Tuesday, Nov 9, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 101

Christopher Marton, Co-Chair
Qinglin Su, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

8:00 Paper 243a: Use of Bayesian Modeling for Failure Risk Analysis and Control Strategy Design — ***Adam Freitag***, *Amanda Rogers, Jose Tabora, Daniel S. Treitler*
8:24 Paper 243b: Accelerated Process Design and Optimization for a Small Molecule COVID-19 Therapeutic — ***Michelle Zheng***, *Rachel Bade, Kevin Stone, Patrick Fier, Gilmar Brito, Steve Castro*
8:48 Paper 243e: A Digital Twin of Flexible Modular Continuous API Manufacturing Process — ***Ravendra Singh***, *Jin-Ping Lim, Nathan Collins, Fernando Muzzio*
9:12 Paper 243f: Quality-By-Control of a Novel Unit for Continuous Integrated Filtration-Drying of Drug Substances — *Francesco Destro, Mesfin Abdi, Xin Feng, Vivian Wang, Erin Wood, Massimiliano Barolo,* ***Zoltan Nagy***
9:36 Paper 185d: Data Pre-Treatment Analysis of Residence Time Distribution (RTD) Profiles for Pharmaceutical Manufacturing Applications — ***Sonia M. Razavi***, *Pooja Bhalode, Andres Roman-Ospino, Huayu Tian, Shashwat Gupta, Atul Dubey, Marianthi Ierapetritou, Fernando Muzzio*

(244) CO2 Capture, Utilization, and Disposal: Key to Clean Energy Production

Tuesday, Nov 9, 8:00 AM
Sheraton Back Bay, Liberty B/C

Chakravarthy Sishtla, Chair
Ambalavanan Jayaraman, Co-Chair

Sponsored by: Transport and Energy Processes

8:00 Paper 244a: Advanced Carbon Capture System for Power Plants— ***Ambalavanan Jayaraman***, *Gokhan Alptekin, David Gribble, Chakravarthy Sishtla*
8:25 Paper 244d: CO_2 Absorption in an Aqueous Amine with a Physical Co-Solvent: Electrolyte NRTL and Rate-Based Process Model and Pilot Plant Experimental Validation. — ***Frederick de Meyer***, *Karen Gonzalez, Louis Boyer, David AlMoucachar, Bénédicte Poulain, Eric Cloarec, Christophe Magnon, Alain Valtz, Christophe Coquelet*
8:50 Paper 244e: The Investigation of Impact of Mineralogical Heterogeneity of Clay–Calcite Based Fracture–Matrix System for CO2 Storage By Using a Hybrid–Scale Model — ***Jiahui You***, *Kyung Jae Lee*
9:15 Paper 244f: Enhancement of Thermal and Hydraulic Characteristics of Microchannel Heat Sinks By Employing sCO_2 As Coolant — *Muhammad Saeed,* ***Abdallah S. Berrouk***, *Munendra Singh*

(245) Cybersecurity and High-Performance Computing in Next-Gen Manufacturing

Tuesday, Nov 9, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 201

Yash Puranik, Chair
Joseph Kwon, Co-Chair

Sponsored by: Next-Gen Manufacturing

8:00 Paper 245a: Control Techniques for Handling Sensor and Actuator Cyberattacks on Evolving Nonlinear Process Systems — ***Henrique Oyama***, *Keshav Kasturi Rangan, Helen Durand*
8:23 Paper 245b: An Algorithm for Exascale-Capable Integrated Process Design and Control — *Nikos Vasilas,* ***Athanasios Papadopoulos***, *Lazaros Papadopoulos, Dimitrios Soudris, Panos Seferlis*
8:46 Paper 245c: Integrated Actuator Attack Detection and Control for Nonlinear Systems Under Lyapunov-Based Economic Model Predictive Control — ***Keshav Kasturi Rangan***, *Henrique Oyama, Helen Durand*
9:09 Paper 245d: Detectability-Based Controller Design Screening for Multiplicative Sensor-Controller Attacks — ***Shilpa Narasimhan***, *Nael El-Farra, Matthew Ellis*
9:32 Paper 245e: Expanding Resilient Lyapunov-Based Economic Model Predictive Control Concepts to a Distributed Control Framework — ***Dominc Messina***, *Henrique Oyama, Helen Durand*

(246) Data-Driven Techniques for Dynamic Modeling, Estimation and Control I

Tuesday, Nov 9, 8:00 AM
Sheraton Back Bay, Back Bay Ballroom D

Joseph Kwon, Chair
Qi Zhang, Co-Chair

Sponsored by: Systems and Process Control

8:00 Paper 246a: Model Predictive Control of Vagus Nerve Stimulation in the Rat Cardiac System Using Long Short-Term Memory Network — ***Andrew Branen***, *Yuyu Yao, Mayuresh V. Kothare, Babak Mahmoudi, Gautam Kumar*
8:19 Paper 246b: High Throughput Characterization of Membrane Transport Properties through Data Analytics — ***Xinhong Liu***, *Jonathan A. Ouimet, Elvis Eugene, William Phillip, Alexander Dowling*
8:38 Paper 246c: Pathologies of Neural Networks As Models of Discrete-Time Dynamical Systems — ***Tianqi Cui***, ***Georgios Psarellis***, *Thomas Bertalan, Sebastian Reich, Ioannis G. Kevrekidis*
8:57 Paper 246d: Data-Driven Dynamic Latent Variable Analysis of Chaotic and Oscillatory Chemical Systems — ***S. Joe Qin***
9:16 Paper 246e: Online Monitoring Based on Reaction Network and Kinetic Model Identification from Spectroscopic Data without *a Priori* knowledge of Species and Reactions — ***Anjana Puliyanda***, ***Karthik Srinivasan***, *Vinay Prasad*
9:35 Paper 246f: Emergent Data-Driven Model Reductions for Coupled, Heterogeneous Agent-Based Systems — ***Thomas Thiem***, *Felix Kemeth, Thomas Bertalan, Carlo R. Laing, Ioannis G. Kevrekidis*
9:54 Paper 246g: Dynamic Operability Analysis Employing Kriging-Based Surrogate Models — ***Victor Alves***, *San Dinh, Fernando V. Lima*
10:13 Paper 246h: Functional Observers for Discrete-Time Nonlinear Systems with Applications to Fault Detection and Estimation — *Sunjeev*

*Venkateswaran,**M.Ziyan Sheriff**, Benjamin Wilhite, Costas Kravaris*

(247) Developments in Extractive Separations: Solvents

Tuesday, Nov 9, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 301

George S. Goff, Chair
David Cantu, Co-Chair

Sponsored by: Extractions

8:00 Paper 247a: Reactive Extraction of (Di-)Carboxylic Acids from Fermentation Broth -Online FTIR for Characterization and Process Control-— ***Lea Nolte**, Christoph Brandenbusch*
8:30 Paper 247b: Solvent-Driven Water Extraction from Hypersaline Brines: Thermodynamics of the Dimethyl Ether System — ***Akshay Deshmukh**, Zi Hao Foo, Caleb C. Stetson, Hyeonseok Lee, Christopher J. Orme, Aaron D. Wilson, John H. Lienhard*
9:00: Break
9:30 Paper 247d: *Computerized Analysis & Optimization of Liquid-Liquid Extraction (CAO-LLE): A Systematic Approach* — ***Andrea Adamo**, Lorenzo Milani*

(248) Developments in Shale Gas and Natural Gas

Tuesday, Nov 9, 8:00 AM
Marriott Copley Place, Fairfield

M R Riazi, Chair
W. Vincent Wilding, Co-Chair
John McLennan, Co-Chair
Fanhua Zeng, Co-Chair
Meng Wang, Co-Chair
Sheima Khatib, Co-Chair
Seiya Hirohama, Co-Chair

Sponsored by: Fuels and Petrochemicals Division

8:00 Paper 248a: CFD and Experimental investigation on Gas-Oil-Water three-phases flow toward the onset of liquid film reversal in a vertical pipe — ***Chuan Xie**, Yonghui Liu, Ning Wu, Jianying Yang, Man Chen, Zhiguo He, Fanhua Zeng*
8:15 Paper 248b: Bog Management during Cargo Unloading at the LNG Regasification Terminal — ***Mohd Shariq Khan**, Wahid Ali, Khursheed B. Ansari*
8:30 Paper 248c: Integrated Cryogenic Upgradation Process for Baseload LNG Plant — ***Ajinkya Pal**, Fares Almomani, Easa Al-Musleh, Iftekhar Karimi*
8:45 Paper 248e: Thermally Induced Two-Step Chemical Looping Process for Hydrogen, Syngas, and Ammonia Production — ***Vinod Amar**, Bharath Maddipudi, Anuradha Shende, Rajesh Shende*

(249) Enabling Technologies Relevant to Drug Substance and Drug Product I

Wednesday, Nov 17, 12:30 PM
Virtual, Pharmaceutical Discovery, Development and Manufacturing Forum (26)

Carla Luciani, Chair
Huiquan Wu, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

12:30 Paper 249g: All vials are not the same: Potential role of vaccine quality in vaccine adverse reactions — ***Bruce Yu**, Marc Taraban, Katharine Briggs*
12:54 Paper 249e: Enabling Agile Process Development and Novel Chemistries through Flow Processes — ***Benjamin Rizkin**, Eric Sacia, Moiz Diwan*
1:18 Paper 249b: A Digital Twin for the L.B. Bohle Tablet Coater — ***Peiyuan Liu**, Kiran S. Iyer, Pankaj Doshi, Alfred Berchielli, Debbie Wanapun, Naomi Hodgins, Sandra Conway, Utkarsh Saxena, Tukaram Suryawanshi, Murtja Khan, Gopal Kasat*
1:42 Paper 308f: Application of Process Modeling and Simulation for Quality Risk Management of Continuous Drug Product Manufacturing — ***Geng Tian**, Abdollah Koolivand, Thomas O'Connor*
2:06 Paper 301e: Implementation of Model-Based Control Strategies in Manufacturing of Drug Substance and Drug Product — ***Stephan Sacher**, Jakob Rehrl, Peter Sagmeister, Julia Kruisz, Rene Lebl, Jason Williams, Ismael Castillo, Selma Celikovic, Martin Sipek, Martin Horn, Oliver Kappe, Johannes G. Khinast*
2:30 Paper 486e: Developing Predictive Models for Degradation of APIs during Hot Melt Extrusion in Pharmaceutical Processes — ***Eric Sacia**, Rachel C. Evans, Russell Hertzler, Moiz Diwan, Andreas Gryczke*

(250) Engineering Strategies to Combat COVID-19

Tuesday, Nov 9, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 108

John Blazeck, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

8:00 Paper 250a: Modeling the Progression of Fibrosis with Dysregulation of ACE2 in COVID19 Patients — ***Mohammad Aminul Islam**, Ashlee Ford Versypt*
8:18 Paper 250b: DNA-Directed Patterning to Validate a Liposome Model of Sars-Cov-2 — ***Molly Kozminsky**, Thomas R. Carey, Lydia L. Sohn*
8:36 Paper 250c: Polymersomes Decorated with Sars-Cov-2 Spike Protein Receptor Binding Domain Elicit Robust Humoral and Cellular Immunity — ***Lisa Volpatti**, Rachel Wallace, Shijie Cao, Michal Raczy, Ruyi Wang, Melody Swartz, Jeffrey A. Hubbell*
8:54 Paper 250d: Inhalation Delivery of RNA-Loaded Lipid Nanoparticles Against Sars-Cov-2 — ***Kai Slaughter**, Daniela Isaacs-Bernal, Ursula Nosi, Eric Donders, Chang Xue, Timothy Cheung, Tekeleselassie Woldemariam, Darryl Falzarano, Amy Wong, Brian Cox, Molly S. Shoichet*
9:12 Paper 250e: A Human Pluripotent Stem Cell Approach to COVID-19 (Invited Speaker) — ***Joyce Chen***
9:48 Paper 250f: Application of Biophysical and Chemical Engineering Principles for Understanding Molecular Scale Interactions Critical to Virus Entry and Infection of Its Host (Invited Speaker) — ***Susan Daniel***

(251) Feedstock Conversion Interface Consortium – Understanding Feedstock Variability to Enable Next Generation Biorefineries (Invited Talks)

Monday, Nov 15, 12:30 PM
Virtual, Sustainable Engineering Forum (23)

Vicki Thompson, Chair
Edward Wolfrum, Co-Chair

Sponsored by: Sustainable Biorefineries

12:30 Paper 251a: Overview of the Fcic — ***Edward Wolfrum***
12:40 Paper 251b: Good Enough for Biotech, Good Enough for Biofuels: A Risk-Based Approach to Managing Biomass Feedstock Variability — ***Beau Hoffman**, Liz Moore, Mark Elless, **Edward Wolfrum***
1:03 Paper 251c: Impact of Material Attributes on Mill Throughput and Performance — ***Jordan Klinger**, Tiasha Bhattacharjee, Neal Yancey, Yidong Xia, Vicki Thompson*
1:26 Paper 251d: Tool Wear Analysis and Mitigation for Various Biomass Comminution Systems — ***Jun Qu**, Kyungjun Lee, Lianshan Li, David Lanning, Jeffrey A. Lacey, George Fenske, Peter Blau, James Keiser, Oyelayo Ajayi, Vicki Thompson*
1:49: Break
2:12 Paper 251f: Advanced Analytical Methodologies Enable Feedstock Screening and Correlation to Pyrolysis Yields and Catalytic Upgrading— ***Steven Rowland**, Calvin Mukarakate, Jordan Klinger, Daniel Carpenter*
2:35 Paper 251g: Biomass Fast Pyrolysis Vapor and Bio-Oil Upgrading: Catalyst Deactivation and Its Correlation with Feedstock Properties — ***Huamin Wang**, Daniel Santosa, Suh-Jane Lee, Igor Kutnyakov*

(252) Fundamentals of Environmental Kinetics and Reaction Engineering

Tuesday, Nov 9, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 309

Rajib Mukherjee, Chair
Matthew Alexander, Co-Chair
Panagiotis Smirniotis, Co-Chair
Hyun-Tae Hwang, Co-Chair

Sponsored by: Fundamentals

8:00 Paper 252a: Abiotic Dehalogenation of 1,4-Dichlorobenenze with Reactive Iron Mineral Coatings in a Contaminated Sediment Core — ***Lisa Axe**, Xin Yin, Han Hua, Wei Ding, Frank Burns, Donna Fennell, James Dyer, Richard Landis*
8:15 Paper 252c: Spatio-Temporal Features of NO_x and Hydrocarbons Trapping and Conversion in a PNA+HCT+OC Sequential Monolith Configuration— ***Abhay Gupta**, Sam Malamis, Michael Harold*
8:30 Paper 252d: Energy-Efficient Nanoparticle Contamination Control Using Functionalized Fiber Filters — ***Laxmicharan Samineni**, Stephanie Velegol, Manish Kumar*

(253) Graduate Student Award: Electronic and Photonic Materials

Tuesday, Nov 9, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 104

Carissa Eisler, Chair
Matthew Crane, Co-Chair

Sponsored by: Electronics and Photonics

8:00 Paper 253a: Exciton Annihilation and Power-Dependent Photoluminescence Quantum Yields of 2D Manganese-Doped Perovskite Nanoplatelets — ***Seung Kyun Ha**, Wenbi Shcherbakov-Wu, Eric Powers, Watcharaphol Paritmongkol, William Tisdale*
8:15 Paper 253b: Temperature Dependent Performance of ITO Schottky Contacts on β- Ga_2O_3 — ***Xinyi Xia**, **Minghan Xian**, Chaker Fares, Fan Ren, Marko Tadjer, Stephen Pearton*
8:30 Paper 253c: The Potential of Solution Processed Silver Indium Diselenide for Photovoltaic Devices — ***David Rokke**, Kyle Weideman, Anna Murray, Rakesh Agrawal*
8:45 Paper 253d: Engineering Energy Flow in Hybrid Plasmonic Systems— ***Steven Chavez**, Suljo Linic*
9:00 Paper 253e: Quantification of Halide Inter-Diffusion in Epitaxially Grown Two-Dimensional Perovskite Lateral Heterostructures — ***Akriti Akriti**, Shuchen Zhang, Zih-Yu Lin, Brett Savoie, Letian Dou*
9:15 Paper 253f: Emergent Optoelectronic Properties through Controlling Nonuniform Charge Carrier Profiles within a Plasmonic Semiconductor Nanocrystal — ***Stephen Gibbs**, Corey Staller, Christopher Dean, Joey Saad, Bharat Tandon, Ankit Agrawal, Delia Milliron*
9:30 Paper 253g: Tunable Photonic Crystals Based on Stabilized Blue Phase Liquid Crystal — ***Sepideh Norouzi**, Monirosadat Sadati*
9:45 Paper 253h: Plasma-Synthesized Gallium Nitride Nanocrystals for Wavelength-Tunable Photoluminescence — ***Dillon Moher**, Elijah Thimsen*
10:00 Paper 253i: Efficient Near-Infrared Emission from Lead-Free Cesium Bismuth Halide Perovskites Doped with Ytterbium — ***Minh Tran**, Iver Cleveland, Greg Pustorino, Eray Aydil*

(254) Honorary Session for John Grace (Invited Talks)

Wednesday, Nov 17, 12:30 PM
Virtual, Particle Technology Forum (03)

Raymond Cocco, Chair
Ah-Hyung Alissa Park, Co-Chair
Xiaotao Bi, Co-Chair

Sponsored by: Fluidization and Fluid-Particle Systems

12:30 Paper 254a: The Lasting Legacy of Prof. John Grace — ***Xiaotao Bi***
12:35 Paper 254b: Relationship between the net electrostatic charge inside a fluidized bed and particles accumulation on the column wall — ***Poupak Mehrani***, *Andrew Sowinski*
12:55 Paper 254c: Numerical study of particle tracking measurements in fluidized bed reactors — ***Tingwen Li***
1:15 Paper 254d: Kinetics & CFD Simulations for Industrial FCC Units— ***Mohammad Abdur Rakib***, *Qi Xu, Zied Soua, Ibrahim A. Abba*
1:35 Paper 254e: CFD-DEM simulation of the onset of fluidization for large particles in a bed of fine sand — *Mohamad Sharei,* ***Farzam Fotovat***
1:55 Paper 254f: Characterization of the main components of fluidization technology applied to thermochemical conversion — ***Sina Tebianian***
2:15 Paper 254g: Experimental investigation of wet pharmaceutical granulation using in-situ synchrotron X-ray imaging — *Chen Li, Yuzhou Zhang, Ning Zhu, Heather Emady,* ***Lifeng Zhang***
2:35 Paper 254h: Solids flux profiles in high velocity CFB risers of FCC catalyst particles — ***Allan Issangya***, *Raymond Cocco, SB Reddy Karri, T. M. Knowlton*
2:55 Paper 254i: Honorary Session for John Grace - Closing — ***Ah-Hyung Alissa Park***

(255) Honorary Session for Prof. Andrew Zydney III

Tuesday, Nov 16, 3:30 PM
Virtual, Separations Division (02)

Ying Li, Co-Chair
Ehsan Espah Borujeni, Co-Chair
Mahsa Rohani, Co-Chair

Sponsored by: Membrane-Based Separations

3:30 Paper 131b: Protein–Membrane Molecular Interactions and Membrane Filtration — *Mirco Sorci, Joseph Hersey, Sal Giglia, Joel Plawsky,* ***Georges Belfort***
3:50 Paper 255a: Constant Flux Viral Reduction Filtration: Effect of Flux on the Retention of Minute Virus of Mice — ***Dharmesh Kanai***
4:10 Paper 131g: Challenges in Membrane Separations during Production of Viral Vectors for Gene Therapy — ***David Bohonak***, *Ying Li*
4:30 Paper 199e: Membrane Chromatography: How Important Is the Device?— ***Raja Ghosh***, *Roxana Roshankhah, Umatheny Umatheva, Guoqiang Chen, Pedram Madadkar, Paul Gatt*
4:50 Paper 255f: The composition of fracturing chemicals plays a key role in membrane fouling by flowback and produced waters from hydraulic fracturing— ***Boya Xiong***, *Andrew Zydney, Manish Kumar*
5:10 Paper 131d: Towards 'perfecting' the Downstream Purification of Therapeutic Viruses — ***David Latulippe***
5:30 Paper 131h: Two Recent Developments in Membranes and Membrane Separations — ***Kamalesh Sirkar***

(256) Hybrid systems, halide perovskites, molecular modeling

Tuesday, Nov 9, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 306

Sapna Sarupria, Chair
Letian Dou, Co-Chair

Sponsored by: Material Interfaces as Energy Solutions

8:00 Paper 256a: Interlayer Vibrational and Thermal Transport Phenomena in 2D Layered Perovskites — ***William Tisdale***
8:25 Paper 256b: Boosting Hybrid 2D Perovskite Stability through Computational Screening of Ligand Chemistries — *Stephen B. Shiring, Zih-Yu Lin,* ***Brett Savoie***
8:50: Break
9:10 Paper 256d: Engineering Entangled Photon Pairs with Metal–Organic Frameworks — *Rubén Fritz,* ***Yamil Colón***, *Felipe Herrera*
9:35 Paper 256e: Invited Talk: A Charge Transfer Framework That Describes Supramolecular Interactions Governing Structure and Properties of 2D Perovskites — ***Melissa Ball***, *Xiaoming Zhao, Arvin Kakekhani, Tianran Liu, Tianran Liu, Andrew Rappe, Y. L. Lynn Loo*
10:00 Paper 256f: Molecular Modeling of Halide Diffusion in 2D Organic-Inorganic Hybrid Perovskites — ***Zih-Yu Lin***, *Akriti ., Shuchen Zhang, Letian Dou, Brett Savoie*

(257) Hydrocarbon Conversion: C1 Aromatization and Coupling

Tuesday, Nov 9, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 205

James W. Harris, Chair
Saurabh Bhandari, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

8:00 Paper 257a: Understanding the Roles of MnO_x, WO_x, and Alkali Metals in the Oxidative Coupling of Methane Using Nanowire-Based Catalysts — ***Divakar Reddy Aireddy***, *Kunlun Ding*
8:18 Paper 257b: Dynamic Study of the Evolution of Metal Species in ZSM-5 during Activation and Reaction in Direct Methane Dehydroaromatization— ***Emanuele Joy***, *Sheima Khatib, Simon Bare, Unmesh Menon, Mustafizur Rahman, Adam Hoffman*
8:36 Paper 257c: High Temperature Methane Pyrolysis in Three-Phase Molten Salt Packed-Bed Reactor — ***Nazanin Rahimi***, *Clarke Palmer, Alexander Stary, Dohyung Kang, Harry Moise, Michael Gordon, Horia Metiu, Eric McFarland*
8:54 Paper 257d: Shaped Catalysts for Oxidative Coupling of Methane— ***Jordan Guillemot***, *Yves Schuurman, David Farrusseng, Thomas Michon*
9:12 Paper 257e: Rate and Reversibility of CH_4 Dehydroaromatization on Mo/H-ZSM-5 — ***Neil Razdan***, *Aditya Bhan*
9:30 Paper 257f: Conversion of Methanol to Hydrocarbons: Why Dienes and Monoenes Contribute Differently to Catalyst Deactivation — ***Zhichen Shi***, *Aditya Bhan*
9:48 Paper 257g: High Temperature Characterization of Reaction Active Sites in Mn-Na_2WO_4/SiO_2 Catalyst for the Oxidative Coupling of Methane — ***Yixiao Wang***, *Sagar Sourav, Matthew. Ross Kunz, Gregory Yablonsky, Rebecca Fushimi*

(258) Hydrogel Biomaterials: Cell Instructive Platforms

Tuesday, Nov 9, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 105

Murat Guvendiren, Chair
Marjan Rafat, Co-Chair
Adam Ekenseair, Co-Chair
Amir Sheikhi, Co-Chair

Sponsored by: Biomaterials

8:00 Paper 258a: Designing Hydrogels with Responsive and Hierarchical Structures for Application As Well-Defined Synthetic Extracellular Matrices— ***April Kloxin***
8:36 Paper 258b: Hydrogels Containing Gradients in Vascular Density Reveal Dose-Dependent Role of Angiocrine Cues on Stem Cell Behavior — ***Mai Ngo***, *Victoria R. Barnhouse, Aidan E. Gilchrist, Brendan A. C. Harley*
8:54 Paper 258c: Investigating Intercellular Interactions in an *in Vitro* 3D Glioblastoma Perivascular Niche Model — ***Rosalyn Hatlen***, *Padmavathy Rajagopalan*
9:12 Paper 258d: Cysteine-Conjugated Thermoresponsive Hydrogels As Mucoadhesive Intestinal Scaffolds — ***Ninad Kanetkar***, *Adam Ekenseair*
9:30 Paper 258e: The Combined Influence of Viscoelastic and Adhesive Cues on Fibroblast Spreading and Focal Adhesion Organization — ***Erica Hui***, *Leandro Moretti, Thomas Barker, Steven Caliari*
9:48 Paper 258f: Using Biomaterials to Maintain Mesenchymal Stem Cell Multipotency and Promote Homogeneous Secretome Production — ***Akram Abbasi***, *Alessia Battigelli, Sachiko Imaichi, Vincent Ling, Anita Shukla*
10:06 Paper 258g: Measuring the Effect of TGF-β and TNF-α on Human Mesenchymal Stem Cell Remodeling of Synthetic Polymer-Peptide Hydrogels Using Multiple Particle Tracking Microrheology — ***John McGlynn***, *Maryam Daviran, Jenna A. Catalano, Hannah E. Knudsen, Kilian J. Druggan, Kiera J. Croland, Amanda Stratton, Kelly Schultz*

(259) In Honor of Professor Venkat Venkatasubramanian's 65th Birthday (Invited Talks)

Tuesday, Nov 9, 8:00 AM
Sheraton Back Bay, Back Bay Ballroom C

Efstratios N. Pistikopoulos, Chair

Sponsored by: Information Management and Intelligent Systems

8:00: Welcoming Remarks
8:05 Paper 259a: Process Safety and AI — ***Warren Seider***
8:25 Paper 259b: Contributions in AI and Applications in Pharmaceutical Engineering — ***Gintaras V. Reklaitis***
8:45 Paper 259c: Revisiting Fault Detection and Diagnosis in the Era of Big Data and Machine Learning — ***Raghunathan Rengaswamy***
9:05 Paper 259d: Process Systems Engineering in the Era of Big-Data and Industry 4.0 Revolution — ***Marianthi Ierapetritou***
9:25 Paper 259e: Smart Process Analytics and Machine Learning — *Weike Sun, Fabian Mohr, Pil Rip Jeon, Moo Sun Hong,* ***Richard D. Braatz***
9:45 Paper 259f: Materials Design Using AI — ***Prasenjeet Ghosh***
10:05 Paper 259g: A Renaissance Man Explores a Societal Problem: A Quantitative Approach to Understanding Fairness in Income Inequality By Venkat Venkatasubramanian — ***Lakshminarayanan Samavedham***, *Suparna Samavedham*
10:25: Concluding Remarks

(260) In Honor of the 2019 Recipient of the Warren K. Lewis Award - Robert H. Davis (Invited Talks)

Tuesday, Nov 9, 8:00 AM
Sheraton Back Bay, Republic Ballroom B

James Medlin, Chair

Sponsored by: Education

8:00 Paper 260a: TBA — ***Kimberly Ogden***
8:20 Paper 260b: High-Throughput Measurement of the Human RED Blood Cell Shear Modulus Distribution As a Function of PO_2 — ***Eric Shaqfeh***, *Juan G. Santiago*
8:40 Paper 260h: Interactive Self-Study Modules for Chemical Engineering Education — ***James Medlin***
9:00 Paper 260d: Combining Scientific Rigor and Outside-the-Box Thinking – Perspectives of a Former Advisee — ***William Bentley***
9:20 Paper 260e: Progress in Therapeutic Biologic Production Technologies and Future Challenges — ***Dana Andersen***
9:40 Paper 260f: Polymers and Light: Towards Advanced, Photoresponsive Materials — ***Christopher Bowman***
10:00 Paper 260g: Comings and Goings of Research and Education in Flow at Small Reynolds Numbers — ***Robert Davis***

(261) In Honor of the 2020 CRE Young Investigator Award Winner (Invited Talks)

Tuesday, Nov 9, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 210

Eranda Nikolla, Chair
Randall Meyer, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

8:00 Paper 261a: Opening Remarks and Welcome to Special Session in Honor of the 2020 CRE YI Award Winner: Phil Christopher — ***Eranda Nikolla***
8:05 Paper 261b: Atomically Dispersed Pt-Group Metal Catalysts: Uniformity, Structural Evolution and Pathways to Increased Functionality — ***Phillip Christopher***
8:40 Paper 261c: Thermodynamic Activity Coefficients Describe the Catalytic Activity of Supported Polyoxometalates — ***Mark Barteau***
9:00 Paper 261d: Characterization of Single Atom Catalysts Using X-Ray Absorption Spectroscopy: Strengths and Pitfalls — ***Simon Bare***
9:20 Paper 261e: An Atomic-Scale View of Single-Site Pt Catalysis for Low-Temperature CO Oxidation — ***E Charles Sykes***
9:40 Paper 261f: Electro-Oxidation Pathways for Biomass-Derived Furans— ***Adam Holewinski***
10:00 Paper 261g: Beyond the Active Site: Controlling the Local Chemical Environment of Active Sites to Achieve Improved Catalytic Performance— ***Suljo Linic***

(262) Microreaction Engineering

Tuesday, Nov 9, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 207

Kishori Deshpande, Chair
Saurabh Bhandari, Co-Chair
Simon Kuhn, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

8:00 Paper 262a: Enhanced Design for Structured Catalytists: 3D Printed Microreactors — ***Oscar Laguna***, *Pablo F. Lietor, Francisco A. Corpas-Iglesias, Cristian Lerma Sr.*
8:21 Paper 262b: Plasma-Liquid Interfacial Interactions in Multiphase Microreactors — ***Kevin Wolf***, *Ryan Hartman*
8:42 Paper 262c: Flow Chemistry-Enabled Extraction Intensification of Switchable Hydrophilicity Solvents — ***Suyong Han***, *Milad Abolhasani*
9:03 Paper 262d: Seamless Scaleup of Continuous Flow Reactor from Lab to 10,000 Metric-Tons Annual Throughput — ***Yi Jiang***, *Qiuyue Ouyang, Yanhua Wang, Wei Shen, Xinjun Wu, Olivier Lobet, Daniela Lavric, Roland Guidat, Sophie Vallon, Alessandra Vizza*
9:24 Paper 262e: Continuous-Flow Synthesis of Antibiotics and Diastereoisomers in Modular Multi-Phase Microfluidic Devices — *Lucie Vobecka, Zdenek Slouka,* ***Michal Pribyl***

(263) Models and Applications of Nuclear Chemical and Separation Processes

Friday, Nov 19, 8:00 AM
Virtual, Nuclear Engineering Division (14)

Reid Peterson, Chair
Wesley H. Woodham, Co-Chair

Sponsored by: Nuclear Engineering Division

8:00 Paper 263a: Adsorption of Organic Iodides from Vessel Off-Gas (VOG) Streams on Silver-Containing Adsorbents — ***Siqi Tang***, *Seungrag Choi, Alexander Wiechert, Austin Ladshaw, Ziheng Shen, Sotira Yiacoumi, Costas Tsouris, Lawrence L. Tavlarides*
8:25 Paper 263b: Hanford Hlw Sludge Processing in Crossflow Filtration— ***Amy Westesen***
8:50 Paper 263c: Application of Blind Source Separation and Partial Least-Squares Regression to Quantify Target Species in Complex Nuclear Waste Mixtures — ***Stefani Kocevska***, *Giovanni Maria Maggioni, Ronald Rousseau, Martha Grover*
9:15 Paper 263e: Interaction with Dark Matter Clusters with Non- Baryonic Particles — ***Suresh Ahuja***

(264) Nanoscale Behavior of Sustainable Processes

Tuesday, Nov 9, 8:00 AM
Marriott Copley Place, Salon J/K

Jindal K. Shah, Chair
Joshua Howe, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

8:00: Break
8:16 Paper 264b: Understanding the Impact of Pore-Polymer Interactions on the Mobility of Poly(ethyleneimine) Confined in Mesoporous SBA-15: Quasi-Elastic Neutron Scattering Studies — ***Hyun June Moon***, *Jan-Michael Y. Carrillo, Johannes Leisen, Christopher W. Jones*
8:32 Paper 264d: Overcoming the Permeability-Selectivity Tradeoff Via the Design of Heterogeneous Pore Wall Chemistries — ***Sally Jiao***, *M. Scott Shell*
8:48 Paper 264e: Hydrogen Bond Patterns of Deep Eutectic Solvents and Non-Deep Eutectic Solvents — ***Joseph Tapia***, *Usman Abbas, Cassie Roberts, Mohammad Selim, Yuxuan Zhang, Qing Shao, Jin Chen, Jian Shi*
9:04: Break
9:20 Paper 264g: Silica-Kaolinite Interface for Shale Gas Application: A Molecular Modeling Study — ***Abdulmujeeb Onawole***, *Mustafa Nasser, Ibnelwaleed Hussein, Mohammed Al-Marri, Ahmad Sakhaee-Pour, Santiago Aparicio*
9:36 Paper 264h: Investigation on the Sodiation of Selenium-Graphene for Na-Ion Batteries: A First-Principles Study — ***Sungwon Park***, *Eunsu Paek*
9:52 Paper 264i: Molecular Insights into the Electrowetting Behavior of Aqueous Ionic Liquid — *Sanchari Bhattacharjee,* ***Sandip Khan***

(265) New Developments in Computational Catalysis I: Method Accuracy and Kinetic Modeling

Tuesday, Nov 9, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 206

Christopher Paolucci, Chair
Paul Meza-Morales, Co-Chair
Eric Walker, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

8:00 Paper 265a: Adsorption Rates and Free Energies Calculations of Methanol-Pt(111) Under Liquid Solvent: Development and Assessment of an Interfacial Force Field — ***Paul Meza-Morales***, *Rachel Getman*
8:20 Paper 265b: Beyond Conventional Transition State Theory in Catalysis: Applications of Matrix Completion Methods — ***Shaama Mallikarjun Sharada***, *Stephen Jon Quiton, Selin Bac, Kareesa Kron*
8:40 Paper 265c: Performance Appraisal of Coverage-Explicit Mean-Field Microkinetic Modelling Strategies — ***Anshuman Goswami***, *William Schneider*
9:00 Paper 265d: Development of Models for Calculation of Elementary Electrochemical Activation Barriers with Density Functional Theory — ***Naveen Agrawal***, *Sharad Maheshwari, Michael J. Janik*
9:20 Paper 265f: When does the choice of DFT functional matter in computational catalysis? The case of methane-to-methanol — ***Vyshnavi Vennelakanti***, *Aditya Nandy, Heather Kulik*
9:40 Paper 265g: Using Reaction Mechanism Generator to Investigate the Catalytic Synthesis of MeOH — ***Christopher Blais***, *Emily Mazeau, Sevy Harris, Su Sun, Maciej Gierada, Eric D. Hermes, Oscar H. Diaz-Ibarra, Cosmin Safta, Eric J. Bylaska, Habib N. Najm, Judit Zádor, C Franklin Goldsmith, Richard H. West*

(266) Novel Nanoparticles and Nanostructured Materials for Pharmaceuticals and Medical Applications

Tuesday, Nov 9, 8:00 AM
Sheraton Back Bay, Hampton

Timothy M. Brenza, Chair

Sponsored by: Nanoparticles

8:00 Paper 266a: Preparation and Evaluation of Hafnium Oxide Nanoparticle CT Contrast Agents — ***Sitong Liu***, *Matthew Po, Bo Yu, Carlos Rinaldi*
8:15: Break
8:30 Paper 266c: Encapsulated Platinum Nanoparticles, Targeted Therapy for Triple Negative Breast Cancer — ***Aida Lopez Ruiz***, *Kathleen McEnnis*
8:45 Paper 266d: Engineering High-Throughput Gold Nanoshell-Liposomes for Effective mRNA Delivery — ***Anisha Veeren***, *Sarah Merkel, Mark Osborn, Joseph Zasadzinski*
9:00 Paper 266e: Fabricating Gold Nanoparticles-Loaded Polyvinyl Alcohol Contact Lens for Laser Protection — ***Zhen Liu***, *Olivia Lanier, Anuj Chauhan*
9:15 Paper 266f: Gold Nanoparticle Synthesis in Contact Lenses for Drug-Less Ocular Cystinosis Treatment — ***Zhen Liu***, *Uday Kompella, Anuj Chauhan*
9:30 Paper 266g: Modulation of Neutrophil Extracellular Trap Formation through Polymer Coating of Metal Oxide Nanoparticles — ***Dhruvi Panchal***, *Esra Al Abazaid, Hunter Snoderly, Celia Martinez de la Torre, Kasey Freshwater, Margaret Bennewitz*

(268) Polymer Viscoelasticity: Mechanics, Processing, and Rheology 2

Tuesday, Nov 9, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 107

Sara Hashmi, Chair
Ralm Ricarte, Co-Chair
Vivek Sharma, Co-Chair
Jeff Ting, Co-Chair

Sponsored by: Polymers

8:00 Paper 268b: Structure and Rheology of Vitrimers Using Dynamic Simulations — *Alessandro Perego,* ***Fardin Khabaz***
8:15 Paper 268c: From Molecular Topology to Viscoelasticity: Predicting the Change of Flow Properties for Entangled Polymers Under Sol-Gel Transition— ***Weizhong Zou***, *Keith Husted, Jeremiah Johnson, Bradley Olsen*
8:30 Paper 268f: Rheology of High Internal Phase Emulsions with Different Interdroplet Interactions — ***Muchu Zhou***, *Reza Foudazi*
8:45 Paper 268g: Nanoscale Morphology and Structural Statistical Mechanics in Kevlar® Fibers Following Ballistic Impact into Multi-Ply Fabric — *Michael Ploch, Kenneth E. Strawhecker,* ***Steven Lustig***
9:00 Paper 268h: Failure Behavior of Polycarbonates Subjected to Ultra-High Strain Rates Impact — *Kyle Callahan, William Heard,* ***Santanu Kundu***
9:15 Paper 268i: Mobility and Recovery of Pressure-Densified and Pressure-Expanded Polystyrene Glass — *Xiao Zhao,* ***Sindee Simon***
9:30 Paper 268a: Strategy for Reducing Molecular Ensemble Size for Efficient Rheological Modeling of Commercial Polymers — ***Yanan Gong***, *Valeriy Ginzburg, Sylvie Vervoort, Jaap Den Doelder, Ronald Larson*
9:45: Break
10:00: Break

(269) Process Design: Innovation for Sustainability

Tuesday, Nov 9, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 311

Vassilis Charitopoulos, Chair

Dharik Mallapragada, Co-Chair
Vikas Khanna, Co-Chair

Sponsored by: Sustainability Science and Engineering

8:00 Paper 269a: Methanol Synthesis Processes — ***Sascha Kleiber***, *Matthaeus Siebenhofer, Susanne Lux*
8:15 Paper 269b: Systematic Approaches for Discovering Innovations to Enable a Sustainable Circular Economy — ***Vyom Thakker***, *Bhavik Bakshi*
8:30 Paper 269c: Shaping the Future with a Hydrogen Value Chain Simulation Platform — ***Ian Willetts***, *Cal Depew*
8:45 Paper 269d: Nutrient Circularity to Abate Nitrogen Pollution: Techno-Economic Assessment of Nitrogen Recovery Systems for Livestock Facilities— ***Edgar Martin Hernandez***, *Gerardo Ruiz-Mercado*, ***Mariano Martin***
9:00: Break
9:15 Paper 269f: Optimal Design of an Open-Cycle Ocean Thermal Energy Conversion System for Energy and Water Supply Considering Multiple-Objectives — ***Ilse María Hernández-Romero***, *Fabricio Nápoles-Rivera, Luis Fabian Fuentes-Cortes, Antonio Flores-Tlacuahuac*

(270) Process Development: Design, Risk Reduction, Implementation and Operations

Tuesday, Nov 9, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 300

Michael Telgenhoff, Chair
Deboleena Chakraborty, Co-Chair
Song Wang, Co-Chair

Sponsored by: Technology Transfer and Manufacturing

8:00 Paper 270f: High Yield and Economical Extraction of Rare Earth and Critical Elements from Coal Ash — ***Bryan E. Sharkey***, *David Gamliel, Dorin V. Preda, Prakash B. Joshi, James C. Hower, Jack Groppo, Todd Beers, Mike Schrock, Brad Perrine, Russell Lambert, Jeffrey Yee*
8:30 Paper 270e: *Gambling on Innovation* — ***Darrell Velegol***
9:00 Paper 270g: Process Development of Organosilicon Compounds— ***Michael Depierro***

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

Tuesday, Nov 9, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 103

Christina Tang, Chair
William Liechty, Co-Chair
Rachel Letteri, Co-Chair

Sponsored by: Polymers

8:00 Paper 271a: My Journey As a Chemical Engineer in Coatings' R&D— ***Anand Atmuri***
8:30 Paper 271b: My Journey into the World of Siloxane Polymerization— ***Pranav Karanjkar***, *Reza Haghpanah, David Tascarella, Kayla Williams, Xiaoyun (Shawn) Chen*
9:00 Paper 271c: Importance of Science and Engineering Fundamentals in My Industrial R&D Career — ***Theresa Whiting***
9:30 Paper 271d: Understanding Charge Transport in Polymeric Encapsulants Enables High Performance, Durable Photovoltaic Devices — ***Brian Habersberger***
10:00 Paper 271e: Structural Color from Synthetic Polymers — ***Matthew Ryan***

(272) PSA/TSA and Adsorption Processes Design and Scale-up

Tuesday, Nov 9, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 305

Roger Whitley, Chair
Celio Cavalcante Jr., Co-Chair
Armin Ebner, Co-Chair
Marcus Mello, Co-Chair

Sponsored by: Adsorption and Ion Exchange

8:00 Paper 272b: Production of Adsorption-based Medical Oxygen Generators: Challenging the Supply Chain in the Corona Pandemic — ***Peter Biedenkopf***
8:19 Paper 272d: Importance of Using Adiabatic Columns for PSA/VSA Pilot Testing and Guidelines for Their Design — ***Guillaume Rodrigues***, *Federico Brandani, David Bigot, Etienne Werlen*
8:38 Paper 615d: Applicability of an Equilibrium Theory Model of a PSA Process Involving Equalization Steps — ***Behnam Fakhari Kisomi***, *Armin Ebner, James A. Ritter*
8:57 Paper 615e: Process Modeling of Temperature Swing Adsorption for Combined Capture and Destruction of VOCs — ***Busuyi Adebayo***, *Fateme Rezaei*
9:16 Paper 615b: PSA Assessment of 3D-Printed Activated Carbon Monoliths for CO_2/CH_4 Separation — *Shane Lawson,* ***Fateme Rezaei***
9:35 Paper 272e: Questions Posed to Adsorption-Based CO_2 Capture — ***Philip Llewellyn***
9:54 Paper 615h: Marrying Materials and Processes: A Superstructure Inspired Optimization Approach for Pressure Swing Adsorption Processes for Pre-Combustion CO_2 Capture — *Amirmohammad Elahi,* ***Sayed Alireza Hosseinzadeh Hejazi***, *Ashwin Kumar Rajagopalan*
10:13 Paper 412b: Continuous Size Fractionation of Nanoparticles Using Magnetic Field Controlled SMB — ***Laura Kuger***, *Carsten-René Arlt, Matthias Franzreb*

(273) Sensors in Startup Companies: Bridging Academia and Industry

Tuesday, Nov 9, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 200

Chelsea Monty-Bromer, Chair

Sponsored by: Sensors

8:00 Paper 273a: Commercialization of Aptamer-Based Electrochemical Sensors — ***Edgar D. Goluch***
8:30 Paper 273b: (Invited Talk) Developing Nanosensor Technology to Detect Cancer in Patients — ***Daniel Heller***, *Zvi Yaari*
9:00 Paper 273e: (Invited Talk) Wearable Health Sensors — ***Chelsea Monty-Bromer***

(274) Special Session In Honor of Arup Chakraborty's 60th Birthday: Statistical Mechanics and Molecular/Materials Modeling

Tuesday, Nov 9, 8:00 AM
Marriott Copley Place, Salon C/D

Bernhardt L. Trout, Chair
Andrew Ferguson, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

8:00 Paper 274a: Data-Driven Protein Engineering Using Deep Representational Active Learning — *Xinran Lian, Nikša Praljak, Rama Ranganathan,* ***Andrew Ferguson***
8:25 Paper 274b: Conformational Landscape of Amyloidal Polypeptides — *Amir H. Saali, Josh Agustin, Harry Ooi, Boris Haimov,* ***Simcha Srebnik***
8:50 Paper 274c: Simulating the Flow of Concentrated Suspensions — *Morton M. Denn,* ***Jeffrey Morris***
9:15 Paper 274d: Multiscale Models for the Kinetics of Polymer Upcycling — *Ryan Yappert, Ziqiu Chen, Damien Guironnet,* ***Baron Peters***
9:40 Paper 274e: Leveraging Nature's Mechanisms to Design Solutions to Engineering Challenges — ***Marc-Olivier Coppens***

(275) Topical Plenary: Topical Conference in Molecular and Materials Data Science (Invited Talks)

Tuesday, Nov 9, 8:00 AM
Marriott Copley Place, Salon H/I

Jim Pfaendtner, Chair
Johannes Hachmann, Co-Chair
Heather Kulik, Co-Chair
Elizabeth Nance, Co-Chair

Sponsored by: Applications of Data Science to Molecules and Materials

8:00: Break
8:25 Paper 275b: Lessons and Opportunities in Data-Driven High Throughput Experimentation — ***Lilo Pozzo***, *Jaime Rodriguez Jr., Sage Scheiwiller, Kacper Lachowski, Maria Politi*
8:50 Paper 275c: Automating Discovery: Accelerating the Search for Novel Perovskites with Robots and Data — ***Joshua Schrier***
9:15 Paper 275d: Streamlining Small Molecule Design and Synthesis— ***Connor Coley***

(276) Tutorial Session on Electrochemical Methods, Systems and Applications (Invited Talks)

Tuesday, Nov 9, 8:00 AM
Sheraton Back Bay, Commonwealth

Ariel Furst, Chair
Christopher Arges, Co-Chair
Matthew Gebbie, Co-Chair
Daniel Esposito, Co-Chair

Sponsored by: Electrochemical Fundamentals

8:00 Paper 276a: Electrochemical Carbon Dioxide Reduction: Overview, Catalysts, and Reactor Designs — ***Kendra Kuhl***
8:35 Paper 276e: From the Synthesis Vial to the Full Cell: Electrochemical Methods for Characterizing Active Materials for Redox Flow Batteries — ***Fikile R. Brushett***
9:10: Break
9:15 Paper 276c: Tutorial on Bioelectrocatalysis for Applications Ranging from Sensing to Energy to Synthesis — ***Shelley Minteer***
9:50 Paper 276d: Fundamentals of Lithium-Sulfur Batteries and Lithium Metal Anode — ***Juchen Guo***

(277) Unit Operations: Experiments, Hands-on Demos and Virtual Labs (In Honor of Deran Hanesian and Angelo Perna's Contributions to Chemical Engineering Education)

Tuesday, Nov 9, 8:00 AM
Sheraton Back Bay, Back Bay Ballroom B

Jennifer Weiser, Chair
Aravind Suresh, Co-Chair
Marya Cokar, Co-Chair

Sponsored by: Undergraduate Education

8:00 Paper 277a: Development and Incorporation of Kit-Based Experiments for Instruction of Fluid and Energy Transfer Laboratory Using Online and Hybrid Teaching Platforms — ***Fernando Mérida Figueróa***, *Spyros Svoronos, Carlos M Rinaldi-Ramos, LiLu Funkenbusch, Sindia M. Rivera-Jimenez*
8:18 Paper 277b: Remote Lab Operations: Development of a Take-Home Lab Kit for the Exploration of Fluid Flow and Pump Characteristics — ***Sandra Pettit***, *Molly Skinner*
8:36 Paper 277c: Combining Experimentation and Simulation in a Unit Operations Lab Course — ***LiLu Funkenbusch***, *Sindia M. Rivera-Jimenez*
8:54 Paper 277d: Gaming for Engineering: Virtual Unit Operation Laboratory Via Unity — ***Ehsan Keyvani***
9:12 Paper 277f: From Nature to the Classroom: Culturing an Environmental Isolate in a Small-Scale Bioreactor for a Unit Operations Laboratory Course— ***Jason Boock***
9:30 Paper 277g: Unit Operations Experiments to Integrate Technologies and Experimental Design in the Curriculum: Mixing Applications — *Andrew Sikora, Justin Friel,* ***Zenaida Otero Gephardt***

9:48 Paper 277h: Strategies for Hands-on Activities in Undergraduate Engineering Curriculum in the Time of COVID-19 Pandemic — ***Gia Huy Pham***, *Cerasela Zoica Dinu*

(278) Waste Valorization

Tuesday, Nov 9, 8:00 AM
Marriott Copley Place, Provincetown

Michael T. Timko, Chair
Justinus Satrio, Co-Chair

Sponsored by: Forest and Plant Bioproducts Division

8:00: Break
8:15 Paper 278b: Heterologous Gene Expression Yields Higher Polyhydroxybutyrate Production in *Paraburkholderia Sacchari* — ***Dianna Long***, *Cheryl Immethun, Mark Wilkins, Rajib Saha*
8:30 Paper 278c: Using Aqueous Renewable Solvents to Recover Lignin from Hybrid Poplar Lignin Cake — ***Carter Fitzgerald***, *Mark Thies*
8:45 Paper 278d: Crystallization of Phosphorus-Incorporated Solids from Liquid Phase of Hydrothermal Carbonization of Cow Manure — ***Saeed Vahed Qaramaleki***, *John Villamil, Angel Fernandez Mohedano, Charles Coronella*

(279) Water Reuse and Recycling II

Tuesday, Nov 9, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 308

Kirti Yenkie, Chair
Toufiq Reza, Co-Chair
Deepak Sharma, Co-Chair

Sponsored by: Water

8:00 Paper 279a: Recent Advances in the Development of Fly Ash Based Geopolymers for the Adsorption of Aqueous-Phase Heavy Metal Contaminants— ***Yusuf Adewuyi***
8:25 Paper 279c: Recovery of High-Value Elements from Produced Water Using Ligand Modified Silica Nanoparticle — *Michael Miranda,* ***Anirban Ghosh***, *Clint Aichele*
8:50 Paper 279d: Development of a Compact, Rapid, and Zero Liquid Discharge Wastewater Treatment System — ***Ramalingam Subramaniam***, *Ian Ivey, Jess Fike*

(280) Water Treatment, Desalination, and Reuse I

Tuesday, Nov 9, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 312

Mahdi Malmali, Co-Chair
Isabel Escobar, Co-Chair
William Phillip, Co-Chair

Sponsored by: Membrane-Based Separations

8:00 Paper 280b: High Recovery Inland Water RO Desalination Via Integration with Continuous Chemically-Enhanced Seeded Precipitation (CCESP) — *Yoram Cohen,* ***Jin Yong Choi***, *Floria Kaufmann*
8:15 Paper 280c: Membrane Distillation of Oil-Contaminated Wastewater Using Novel Fouling-Resistant Janus Membranes — ***Mengfan Zhu***, *Yu Mao*
8:30 Paper 280d: A New Emulsion Liquid Membrane (ELM) Enhanced By Nanoparticles and Ionic Liquid for Recovering Heavy Metals from Wastewater Using a Vanadium Compound As Example. — ***Qusay Al-Obaidi***, *Muthanna M. Aldahhan*
8:45 Paper 280e: Selective and Continuous Lead Removal By Shock Electrodialysis Device — ***Huanhuan Tian***, *Mohammad A. Alkhadra, Kameron Conforti, Martin Z. Bazant*
9:00 Paper 280f: Facile Size-Selective Defect Sealing in Large-Area Atomically Thin Graphene Membranes for Sub-Nanometer Scale Separations — ***Piran Kidambi***
9:15 Paper 280g: MF and UF Coated Membranes for Selective Separation of Organic Anions-Pfas — ***Francisco Leniz***, *Dibakar Bhattacharyya, Ronald Vogler, Phillip Sandman, Natalie Harris*
9:30 Paper 403b: Sub-10 Nm Glassy Amorphous Perfluoropolymers for Desalination and Solvent Dehydration. — ***Ameya Tandel***, *Haiqing Lin*

(281) MFF/MAC Real Talk: Navigating the Academic Career Path for Influence, Impact and Success

Tuesday, Nov 9, 11:00 AM
John B. Hynes Veterans Memorial Convention Center, 202

Reginald Rogers Jr., Chair
Jude Phillip, Co-Chair

Sponsored by: Minority Affairs Committee (MAC)

(282) Andreas Acrivos Award for Professional Progress in Chemical Engineering Lecture

Tuesday, Nov 9, 11:15 AM
John B. Hynes Veterans Memorial Convention Center, Ballroom B

Michael Strano, Chair

Sponsored by: Awards Committee

11:15 Paper 282a: Directed Evolution of New Adeno-Associated Viral Vectors for Clinical Gene Therapy — ***David V. Schaffer***

(283) Advances in bioseparations

Tuesday, Nov 9, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 303

Cristiana Boi, Chair
Piran Kidambi, Co-Chair

Sponsored by: Bio Separations

12:30 Paper 283a: Leveraging First Principles to Advance Downstream Process Development and Understanding for Biologics — ***Jennifer Pollard***
1:10 Paper 283b: *In silico* Development of Chromatography Processes Using Orthogonally Selective Multimodal Resins — ***Nicholas Vecchiarello***, *Camille Bilodeau, Steven Cramer*
1:30 Paper 283c: Effective Property Prediction for Solvent Design and Bioproduct Extraction — ***Jianping Li***, *Christos Maravelias, Reid Van Lehn*
1:50 Paper 283e: Rapid Selection of Optimal Systems for Aqueous Two-Phase Extraction - Using Excipients to Increase Solubility and Stability of High-Value Biomolecules - — ***Maximilian Wessner***, *Christoph Brandenbusch*

(284) Advances in Computational Methods and Numerical Analysis II

Tuesday, Nov 9, 12:30 PM
Sheraton Back Bay, Independence Ballroom East

Matthew Stuber, Chair
Rajib Saha, Co-Chair

Sponsored by: Applied Mathematics and Numerical Analysis

12:30 Paper 284a: Introducing a Pair of Tools for the *in silico* Design and Dynamic Simulation of Eukaryotic Genetic Circuits — ***Wheaton Schroeder***, *Rajib Saha*
12:49 Paper 284b: Control Invariant Set Computation for Nonlinear Systems: A Distributed Approach — ***Benjamin Decardi-Nelson***, *Jinfeng Liu*
1:08 Paper 284c: Accurate Surrogate Models for Stochastic Simulations— ***Samira Mohammadi***, *Selen Cremaschi*
1:27 Paper 284e: Quantimpy: Minkowski Functionals and Functions with Python— ***Arnout Boelens***, *Hamdi Tchelepi*
1:46 Paper 284f: Accelerate Simulations of Multivalent Letin-Glycan Binding Process through Hybrid PDE-Kinetic Monte Carlo Model — ***Dongheon Lee***, *Aaron Green, Hung-Jen Wu, Joseph Kwon*
2:05 Paper 284d: New and Efficient Interval Sampling Methods for P-Box Uncertainties — ***Urmila Diwekar***, ***Philips Kochumuriel***, *Mark A. Stadtherr*
2:24 Paper 284g: Model Free Adaptive Control of the Failing Heart Managed By Mechanical Supporting Devices — ***Jeongeun Son***, *Yuncheng Du*
2:43 Paper 284h: Emergent Evolution Equations from (multi-)Puzzle Tiles, with a *Drosophila* Embryonic Development Example — ***David Sroczynski***, *Felix Kemeth, Stanislav Y. Shvartsman, Ronald Coifman, Ioannis G. Kevrekidis*

(285) Advances in Fluid Particle Separations

Tuesday, Nov 9, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 301

Isaac Gamwo, Chair
Seyi Odueyungbo, Co-Chair

Sponsored by: Fluid-Particle Separations

12:30 Paper 285a: Development of Enclosed Space Membrane Air Filtration for Viral Aerosol Capture and Deactivation — ***Kevin Baldridge***, *Kearstin Edmonds, Rollie Mills, Thomas D. Dziubla, J. Zach Hilt, Rebecca Dutch, Dibakar Bhattacharyya*
12:55: Break
1:20 Paper 285c: Compaction of Compressible Filter Cakes By Applying Low Pressure and Oscillatory Shear — ***Tolga Yildiz***, *Marco Gleiss, Hermann Nirschl*
1:45 Paper 285d: Self-Assembly and Sedimentation of Superparamagnetic Iron Oxide Nanoparticles Using Enhanced Quadrupole Magnetic Sorters — ***Xian WU***, *Jenifer Gómez-Pastora, Jeffrey Chalmers*

(286) Advances in Low-Cost Renewable Hydrogen Production at Large Scale

Thursday, Nov 18, 8:00 AM
Virtual, Synthetic & Renewable Fuels (TH)

Eric Miller, Chair
William Gibbons, Co-Chair

Sponsored by: Synthetic & Renewable Fuels

8:00 Paper 286a: Green Hydrogen – Removing Hurdles and Creating the Right Incentives to Make It Viable — ***Achim Wechsung***, *Michael Orella, Michael Stern, Harri Kytomaa*
8:15 Paper 286b: A Coating Strategy for Stable H_2 Production from Semiconductor Particles — ***Shu Hu***, *Rito Yanagi, Tianshuo Zhao, Jake Heinlein*
8:30 Paper 286c: Nickel Ferrite - Ceria Composites for Solar Thermochemical Fuel Production – Efficiency Analysis and Design Goals — ***Aniket Patankar***, *Xiaoyu Wu, Wonjae Choi, Harrry Tuller, Ahmed F. Ghoniem*
8:45 Paper 286e: Boosting Electroreduction Kinetics of Nitrogen to Ammonia Viatuning Electron Distribution of Single-Atomic Iron Sites — ***Yan Li***, ***Yang Hou***

(287) Advances in Machine Learning and Intelligent Systems II

Tuesday, Nov 9, 12:30 PM
Sheraton Back Bay, Independence Ballroom West

Alexander Dowling, Chair
Antonio del Rio Chanona, Co-Chair

Sponsored by: Information Management and Intelligent Systems

12:30 Paper 287a: Machine Learning for Process Applications in Cement Industries — *Christos Chatzilenas,* ***Thanasis Gentimis***, *Antonios Kokosis,* ***Theodore Dalamagas***
12:49 Paper 287b: Deep Learning Tools for Dense Fluorescent Microscopic Images and *C. Elegans* Whole-Brain Imaging — ***Shivesh Chaudhary***, *Hang Lu*
1:08 Paper 287c: Machine Learning to Speed up Dynamic Flux Balance Analysis (FBA) and FBA-Based Reactive Transport Simulations — ***Hyun-Seob Song***, *Joon-Yong Lee, William Nelson, Christopher S. Henry,*

Janaka N. Edirisinghe, J. David Moulton, Xingyuan Chen, Timothy Scheibe
1:27 Paper 287d: Coarse-Grained Dynamics for Epidemics on Adaptive Networks — ***Tianqi Cui**, Alexei Makeev, Thomas Bertalan, Ioannis G. Kevrekidis*
1:46 Paper 287e: Explainable AI: Generating Causal Explanations of Machine Learning-Derived Models from Data — ***Abhishek Sivaram**, Venkat Venkatasubramanian*
2:05 Paper 287f: Data-Driven Multi-Stage Stochastic Optimization on Time Series — ***Rohit Kannan**, Nam Ho-Nguyen, James Luedtke*
2:24 Paper 287g: Learning Decision-Making Models Via Data-Driven Inverse Optimization — ***Rishabh Gupta**, Qi Zhang*
2:43 Paper 287h: Simultaneous Planning and Scheduling Under Demand Uncertainty for Multi-Product Systems Using Data-Driven Bi-Level Optimization— ***Burcu Beykal**, Styliani Avraamidou, Efstratios N. Pistikopoulos*

(288) Advances in Metabolic Engineering-Prokaryotic Organisms

Tuesday, Nov 9, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 111

Arul Mozhy Varman, Chair
Andrew Jones, Co-Chair

Sponsored by: Bioengineering

12:30 Paper 288a: A New-to-Nature Metabolic Pathway for Methanol and Formaldehyde Assimilation in *Escherichia coli* — ***Seung Hwan Lee**, Alexander Chou, Fayin Zhu, James M. Clomburg, Ramon Gonzalez*
12:48 Paper 288b: Microbial Synthesis of Chondroitin Sulfates and N-Glycolyl Chondroitin Using Engineered *Escherichia coli.* — ***Adeola Awofiranye**, Abinaya Badri, Asher J. Williams, Ke Xia, Payel Datta, Keith Fraser, Wenqin He, Sultan N. Baytas, Robert J. Linhardt, Mattheos Koffas*
1:06 Paper 288c: Production of Psilocybin and Norbaeocystin in *E. coli* Enable the Discovery of an Entourage Effect in *Psilocybe,* "Magic", Mushrooms— ***Alexandra Adams**, Nicholas Anas, Abhishek Sen, Matthew McMurray, Andrew Jones*
1:24 Paper 288d: Complementary Enzyme and Metabolic Engineering Strategies for Highly Selective Oleochemical Bioprocesses — ***Michael A. Jindra**, Brian Pfleger*
1:42 Paper 288e: A Genome-Scale Metabolic Model of *Anabaena* Sp. ATCC 33047 and Its Application to Design Strategies to Overproduce Nylon Monomers— ***John I Hendry**, Hoang Dinh, Debolina Sarkar, Lin Wang, Anindita Bandyopadhyay, Himadri B Pakrasi, Costas D. Maranas*
2:00 Paper 288f: Substrate-Activated Expression of a Biosynthetic Pathway in *Escherichia coli* — ***Cynthia Ni**, Kevin J. Fox, Kristala Prather*
2:18 Paper 288g: Characterize and Release Biological Constraints for Lignocellulose Bioconversion — ***Xuan Wang***

(290) Applications of Data Science in Catalysis and Reaction Engineering II

Tuesday, Nov 9, 12:30 PM
Marriott Copley Place, Salon H/I

Zachary Ulissi, Chair
Bryan Goldsmith, Co-Chair
Thomas Senftle, Co-Chair

Sponsored by: Applications of Data Science to Molecules and Materials

12:30 Paper 290a: Building Catalytic Descriptors with Iterative Bayesian Additive Regression Trees (iBART) — ***Chun-Yen Liu**, Shengbin Ye, Meng Li, Thomas Senftle*
12:45 Paper 290b: Unsupervised Machine Learning to Extract the Electronic and Chemical Properties of Alloy and Metal Oxide Surfaces — ***Jacques Esterhuizen**, Bryan Goldsmith, Suljo Linic*

(291) Area Plenary 1: Emerging Areas in Polymer Science and Engineering (Invited Talks)

Tuesday, Nov 9, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 103

Siamak Nejati, Chair
Mingjiang Zhong, Co-Chair

Sponsored by: Polymers

12:30 Paper 291a: Naming, Classifying, and Comparing Polymers in the Era of Data Science — ***Bradley Olsen***
1:00 Paper 291b: The Relaxation Times of Polyelectrolyte Complexes and Their Correlation to Water and Ion-Pairing — ***Jodie Lutkenhaus***
1:30 Paper 291c: Multiscale Simulation of Flow-Induced Crystallization in Polymers — *David A. Nicholson, Marat Andreev, Chinmay Gangal,* ***Gregory Rutledge***
2:00 Paper 291d: Macromolecular Engineering of Formulations: Rheology, Stringiness, Spinnability, and Printability — ***Vivek Sharma***
2:30 Paper 291e: Challenges and Limitations of SEC for the Characterization of Polymers — *Dylan Walsh, Yash Laxman Kamble,* ***Damien Guironnet***

(292) Area Plenary: Adsorption and Ion Exchange - In Honor of Prof. Stefano Brandani (Invited Talks)

Tuesday, Nov 9, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 305

Peter Ravikovitch, Chair
F Handan Tezel, Co-Chair

Sponsored by: Adsorption and Ion Exchange

12:30 Paper 292g: Diffusion in Nanoporous Materials: Challenges, Surprises and Tasks of the Day — ***Jörg Kärger***
12:52 Paper 292a: Diffusion mechanism of CO_2 in zeolite 5A pellets — *Hyungwoong Ahn, Maria-Chiara Ferrari, Daniel Friedrich, Mauro Luberti, Giulio Santori,* ***Enzo Mangano***
1:10 Paper 292b: Brandani Honorary Session Invited Talk 2 Placeholder— ***James A. Ritter***
1:28 Paper 292c: Helium Recovery from Dilute Sources — ***Jeffrey R. Hufton***
1:46 Paper 292d: Adsorption and phase behaviour of CO_2 and CH_4 in hierarchically organized nanoporous materials over a wide range of temperatures and pressures — *Peter Leicht,* ***Matthias Thommes***
2:04 Paper 292e: Brandani Honorary Session Invited Talk 5 Placeholder— ***Federico Brandani***
2:22 Paper 292f: Performance-based screening of porous materials for carbon capture — ***Lev Sarkisov***
2:40 Paper 292h: Brandani Honorary Session Invited Talk 8 Placeholder— ***Celio Cavalcante Jr.***

(293) Biomanufacturing with Advanced Bioreactor and Bioprocess Engineering

Tuesday, Nov 9, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 110

Dongming Xie, Chair
Amol Janorkar, Co-Chair

Sponsored by: Bioengineering

12:30 Paper 293a: Continuous Cell Production Using a Multiphase Bioreactor with Optimized Spiroid — ***Rithvija Avvari**, Paul W. Todd, Thomas R. Hanley*
12:51 Paper 293b: Development of a Novel Centrifugal Bioreactor with a Real-Time Monitoring Sensor for T Cell Exhaustion with Applications in Cancer Immunotherapy — ***Brenden Fraser-Hevlin**, Kitana Kaiphanliam, William C. Davis, Bernard Van Wie*
1:12 Paper 293c: Biomanufacturing and Testbed Development for the Continuous Production of Monoclonal Antibodies — ***Dragana Bozinovski**, Elizabeth M. Cummings Bende, Andrew J. Maloney, Jose Sangerman, Alexis B. Dubs, Amos E. Lu, Moo Sun Hong, Nili Persits, Anastasia Artamonova, Rui Wen Ou, Weike Sun, Jacqueline Wolfrum, Paul W. Barone, Rajeev J. Ram, Stacy L. Springs, Richard D. Braatz, Anthony J. Sinskey*
1:33 Paper 293d: Application of a Raman Spectroscopy Analyzer and Process Data Analytics Tools to Enable in-Line Monitoring of Perfusion Mammalian Cell Cultures — ***Ricardo Suarez Heredia**, Amy Wood, Alison Dupont, Gabriela Hall, Hiral Gami, Haley Matthews, Johan Cailletaud, Celia Sanchez, Charlotte Javalet, Mikhail Kozlov*
1:54 Paper 293e: Optimizing T Cell Growth in a Centrifugal Fluidized Expansion (CentriFLEX) Bioreactor through Kinetic Growth Models — ***Kitana Kaiphanliam**, Brenden Fraser-Hevlin, William C. Davis, Bernard Van Wie*
2:15 Paper 293f: Model-Based Design of Recombinant Adeno-Associated Viral Vector Production — ***Tam Nguyen**, Sha Sha, Paul W. Barone, Caleb Neufeld, Jacqueline Wolfrum, Stacy L. Springs, Anthony J. Sinskey, Richard D. Braatz*
2:36 Paper 293g: Synthetic Pathways for the Microbial Production of Isoprenoids, Polyketides, and Prenylated Aromatics — ***Ramon Gonzalez***

(294) Biomimetic Materials II

Tuesday, Nov 9, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 209

R. Helen Zha, Chair
Handan Acar, Co-Chair
Xi Chen, Co-Chair
Nader Taheri-Qazvini, Co-Chair

Sponsored by: Biomaterials

12:30 Paper 294a: Development of Peptoid-Based Materials to Control Hydrogel Mechanics and Degradation in Artificial Extracellular Matrices— ***Adrianne Rosales**, Mariah Austin, Logan Morton, Hattie Schunk*
12:48 Paper 294c: Engineered Matrices with Dynamic Crosslinks Support the Culture of Human Neural Progenitor Cells — ***Michelle Huang**, Julien G. Roth, Sarah C. Heilshorn*
1:06 Paper 294d: Mimicking Nacre through Magnetically Driven Self-Assembly of Colloids — ***Joelle Medinger**, Marco Lattuada*
1:24 Paper 294e: Biomineralization By Design: Application of *De Novo* Proteins for Nanocrystal Synthesis — ***Leah Spangler**, Michael H. Hecht, Gregory D. Scholes*
1:42 Paper 294f: A Hydrogel/Particle-Based Biomimetic Material System for Assay and Solid-State NMR Spectroscopy of Biomembranes and Soft Materials— ***Malcolm Lane Gilchrist**, Robert Messinger*
2:00 Paper 294g: Compression-Induced Stiffening in Biopolymer Networks with Embedded Particles — ***Jordan Shivers**, Jingchen Feng, Anne van Oosten, Herbert Levine, Paul A. Janmey, Fred MacKintosh*
2:18 Paper 294h: Cavitation Pressure Limit of Water Confined in Bio-Mimetic Water-Responsive Structures — ***Zhi-Lun Liu**, Xi Chen*

(295) Biomimetic Structures and Biomolecular Self-Assembly

Tuesday, Nov 9, 12:30 PM
Marriott Copley Place, Simmons

Anju Gupta, Chair
Alexander Marras, Co-Chair

Sponsored by: Bionanotechnology

12:30 Paper 295a: Biotemplating of Barley Stripe Mosaic Virus Virus-like Particles for Directed Synthesis of Metal Nanomaterials — ***Yu-Hsuan Lee**, Kok Zhi Lee, Shohreh Hemmati, Sue Loesch-Fries, Kevin Solomon, Michael T. Harris*

12:53 Paper 295b: Metal-Organic Frameworks for Vaccine Stabilization: A Translational and Mechanistic Study — ***Rohan Murty***, *Mrinal Bera, Krista Walton, Mark R. Prausnitz*
1:16 Paper 295d: DNA-Caged Polymer Micelles for Cell and Tissue Labeling— ***Elizabeth Jergens***, *Jessica Winter*
1:39 Paper 295e: DNA Origami Tubes with Reconfigurable Cross-Sections— ***Anjelica Kucinic***, *Chao-min Huang, Jingyuan Wang, Carlos E. Castro*
2:02 Paper 295f: CRISPR/Cas-Directed Hierarchical Assembly of Protein-DNA Hybrid Nanostructures — ***Joshua Hubbard***, *Samuel Lim, Minghui Liu, Markita Landry, Nicholas Stephanopoulos, Douglas S. Clark*
2:25 Paper 26e: In-Situ Monitoring with a Surface Plasmonic Enhanced Native Fluorescence in the Ultraviolet Spectral Region — ***Ji-Young Lee***, *Yunshan Wang*
2:48: Break

(296) Catalysis on Low Dimensional Materials II

Tuesday, Nov 9, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 203

Craig Plaisance, Chair
Ian McCrum, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

12:30 Paper 296a: Electrifying CO2 into Pure Liquid Fuels — ***Haotian Wang***
1:00 Paper 296b: Role of Defects on CoO_x nanoparticle Structure and Water Splitting Activity — ***Anthony Curto***, *Zhaozong Sun, Jeppe Lauritsen, Aleksandra Vojvodic*
1:20 Paper 296c: Active Phases, Reaction Centers and Catalytic Mechanism of Ni-Based and Co-Based Layered Double Hydroxides for the Oxygen Evolution Reaction — ***Zhenhua Zeng***, *Jeffrey Greeley*
1:40 Paper 296e: Ethane Dehydrogenation over Metal Loaded Two-Dimensional Zeolite Catalysts — *Ying Pan, Antara Bhowmick,* ***Dongxia Liu***
2:00 Paper 296f: Correlating Structural and Electronic Properties of Ultra-Small, Atomically Precise Nanostructures with Electrocatalysis — ***Anantha Venkataraman Nagarajan***, *Michael Cowan, Malena Rybacki, Ethan Holbrook, Julia McKay, Giannis Mpourmpakis*
2:20 Paper 296g: Hydrolysis of Phosphoric Acid Supported on Silica Bilayers/Ru(0001) — ***Matheus Dorneles de Mello***, *Sai Praneet Batchu, Stavros Caratzoulas, Dionisios Vlachos, Michael Tsapatsis, Jorge Boscoboinik*

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

Wednesday, Nov 17, 3:30 PM
Virtual, Entrepreneurship in Chemical Engineering (T2)

Mark Vreeke, Chair
William Byers, Co-Chair

Sponsored by: Entrepreneurship in Chemical Engineering

(298) Colloidal Dispersions

Tuesday, Nov 9, 12:30 PM
Sheraton Back Bay, Back Bay Ballroom A

Carlos Silvera Batista, Chair
Mark Kastantin, Co-Chair
Ubaldo M. Córdova-Figueroa, Co-Chair

Sponsored by: Interfacial Phenomena

12:30 Paper 298a: Flash Nanoprecipitation of Ionomers for the Scalable Production of Salt-Responsive Pickering Emulsifiers — ***Douglas Scott***, *Robert K. Prud'homme, Rodney Priestley*
12:50 Paper 298b: Preventing Buckling in Drying Suspensions of Anisotropic Particles — ***Ahmed Al Harraq***, *Bhuvnesh Bharti*
1:10 Paper 298c: Liquid Crystal Emulsions Stabilized By Nanoparticle-Surfactant Complexes — ***Oscar H. Piñeres-Quiñones***, *David M. Lynn, Claribel Acevedo-Velez*
1:30 Paper 298e: Comparison Analysis of 2D Nanomaterial Dispersions Partitioned By Differential Sedimentation Using Analytical Ultracentrifugation and Microscopy Methods — *Christopher Sims, Elisabeth Mansfield, Jason P. Killgore,* ***Jeffrey Fagan***
1:50 Paper 298f: Effects of the Method of Preparation and Dispersion Media on the Optical Properties and Particle Sizes of Aqueous Dispersions of Didodecyldimethylammonium Bromide (DDAB) — ***An-Hsuan Hsieh***, *Elias I. Franses, David Corti*

(299) Computational Approaches for Studies at the Nanoscale

Tuesday, Nov 9, 12:30 PM
Marriott Copley Place, Wellesley

Sasan Nouranian, Chair

Sponsored by: Nanoscale Science and Engineering Forum

12:30: Break
12:50 Paper 114a: Data Management Schema Design for Effective Nanoparticle Formulation for Probing and Treating Neurological Disease — ***Hawley Helmbrecht***, *Andrea Joseph, Rick Liao, Nuo Xu, Chih-Chung Chen, Elizabeth Nance*
1:10 Paper 299c: Molecular Dynamics Simulation of the Sintering of Titanium/Aluminum Core/Shell Nanoparticles — *Huadian Zhang, Jungmin Jeon, Farzin Rahmani,* ***Sasan Nouranian***, *Shan Jiang*
1:30 Paper 299d: Elucidating the Molecular Mechanism of Diffusive and Electrophoretic Ion Transport Under Single Digit Nanoconfinement — ***Rahul Prasanna Misra***, *Zhongwu Li, Aleksandr Noy, Daniel Blankschtein*
1:50 Paper 299e: High-Throughput Computational Analysis of the Role of Finite Temperature in the Optical Response of 2D Materials — ***Anubhab Haldar***, *Tianlun Allan Huang, Quentin Clark, Sahar Sharifzadeh*
2:10 Paper 299f: *Ab Initio* Molecular Dynamics Simulations of the Hydration of Zwitterions — ***Pranab Sarker***, *Md Symon Jahan Sajib, Tao Wei*

(300) Concentrated Solar Power Generation and Chemical Processing II

Tuesday, Nov 9, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 313

Christopher L. Muhich, Chair
Nick AuYeung, Co-Chair
Alexandre Yokochi, Co-Chair
Ashley Pennington, Co-Chair
Wojciech Lipinski, Co-Chair

Sponsored by: Sustainable Energy

12:30 Paper 300a: Experiment Investigation of a Solar Reactor for Thermochemical Syngas Production Via the CeO_2-CH_4-CO_2 Hybrid Redox Cycle in a Concentrating Solar Tower — ***Mario Zuber***, *Moritz Patriarca, Simon Ackermann, Philipp Furler, Manuel Romero, José González, Aldo Steinfeld*
12:51: Break
1:12 Paper 300c: Solar Syngas Production from H_2O and CO_2 Applicable for Methanol or Fischer-Tropsch Synthesis — ***Remo Schäppi***, *Philipp Haueter, Philipp Furler, Aldo Steinfeld*
1:33 Paper 300d: Rotary Kilns: A Powerful and Effective Tool for Running Particle-Based Solar-Chemical Processes — ***Martin Roeb***
1:54 Paper 300e: Performance of a Concentrated Solar–Gliding Arc Plasma Reactor for CO_2 Decomposition: Effect of Catalyst Monolith — ***Visal Veng***, *Benard Tabu, Heba Ahmed, Hsi-Wu Wong, Juan Trelles*
2:15 Paper 300f: High-Temperature Heat Recovery System Coupled to a Solar Reactor for Thermochemical Redox Splitting H_2O and CO_2 — ***Alon Lidor***, *Jamina Häseli, Yves Aschwanden, Philipp Haueter, Aldo Steinfeld*
2:36 Paper 300g: Modelling and Chemical Compatibility of Super-Critical Carbon Dioxide Flow in Micro-Channels of Microvascular Carbon/Carbon Composites — ***Jose Cordeiro Jr.***, *Hema Ramsurn, Daniel W. Crunkleton, Todd Otanicar, Michael Keller*

(301) Control Strategies in Pharmaceutical Development and Manufacturing II

Tuesday, Nov 9, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 101

Christopher Marton, Co-Chair
Qinglin Su, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

12:30 Paper 301a: The Use of Linear Regression and R^2 in Continuous Manufacturing to Dictate When Loss-in-Weight Data Is Acceptable to Control Feeding Following Feeder Refill — ***Brian Krieg***, *Jesus Torres, Keirnan LaMarche*
12:54 Paper 301b: Continuous Manufacturing Control Strategy for Material Traceability — ***Efrain Aymat***
1:18 Paper 301c: Development of a High-Fidelity Digital Twin Using DEM for Evaluating Continuous Manufacturing Control Approaches — ***Dalibor Jajcevic***, *Johan Remmelgas, Peter Toson, Marko Matic, Theresa R. Hörmann-Kincses, Michela Beretta, Jakob Rehrl, Thomas O'Connor, Abdollah Koolivand, Geng Tian, Scott M. Krull, Johannes G. Khinast*
1:42 Paper 301d: RTD Based Digital Twin of Continuous Pharmaceutical Manufacturing Process — ***Ravendra Singh***, *Fernando Muzzio*
2:06 Paper 301f: New Methods for Design Space Identification and a Re-Interpretation of ICH Endorsed Guide for Q8Q9Q10 Implementation — ***Salvador Garcia-Munoz***

(302) Crystallization of Pharmaceutical and Biological Molecules

Tuesday, Nov 9, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 302

Marina Tsianou, Chair
Haitao Zhang, Co-Chair
Manish Kelkar, Co-Chair

Sponsored by: Crystallization and Evaporation

12:30: Welcoming Remarks
12:35 Paper 302a: Molecular Simulations Unravel the Dynamics of Oiling out of β-Alanine — ***Prem Kumar Reddy Podupu***, *Anish Dighe, Paria Coliaie, Meenesh Singh*
12:55 Paper 302b: New Insights on the Effects of Molecular Rigidity and Purity on Crystallization Pathways — ***Lotfi Derdour***, *John L. Woodard*
1:15 Paper 302c: Protein Crystallization with Gas Bubble Templates and Scaling-up Studies — ***Wenqing Tian***, *Huaiyu Yang, Chris D. Rielly*
1:35: Break
1:55 Paper 302e: Crystallization Development for Molnupiravir, an Investigational Antiviral for the Treatment of COVID-19 — ***Rachel Bade***, *Michelle Zheng, Marc Poirer, Gilmar Brito, Eric Sirota, Jameson Bothe, Darryl Chang, Plamen Grigorov, Michael Ward, Yingju Xu, Patrick Fier*
2:15 Paper 302f: An Experimental Study on the Ice Nucleation Properties of Aqueous Solutions in Vial Freezing Processes — ***Leif-Thore Deck***, *Marco Mazzotti*

(303) Data-Driven Techniques for Dynamic Modeling, Estimation and Control II

Tuesday, Nov 9, 12:30 PM
Sheraton Back Bay, Back Bay Ballroom D

Qi Zhang, Chair
Joseph Kwon, Co-Chair

Sponsored by: Systems and Process Control

12:30 Paper 303a: Data-Driven Development of Approximate Inertial Forms and Closures for Coarse-Scale Modeling of Multiphase Flows — ***Cristina Martin Linares***, *Thomas Bertalan, Seungjoon Lee, Jiacai Lu, Gretar Tryggvason, Ioannis G. Kevrekidis*
12:49 Paper 303b: Combining Particle-Based Simulations and Machine Learning Models for the Prediction of Defect Kinetics in Thin Films of Symmetric Diblock Copolymers — ***Ludwig Schneider***, *Juan J. de Pablo*
1:08 Paper 303c: Machine Learning-Based Predictive Control of Nonlinear Parabolic PDE Systems — ***Aarsh Dodhia***, *Zhe Wu, Panagiotis D. Christofides*
1:27 Paper 303d: Symmetry Reduction for Deep Reinforcement Learning Active Flow Control of Chaotic Spatiotemporal Dynamics — ***Kevin Zeng***, *Michael Graham*
1:46 Paper 303e: Ensuring Convexity in Constrained Optimal Control Using Input Convex Neural Networks — ***Shu Yang***, *B Wayne Bequette*
2:05 Paper 303f: Initializing the Internal States of Lstm Neural Networks Via Manifold Learning — *Felix Kemeth, Thomas Bertalan, Nikolaos Evangelou, Tianqi Cui,* ***Saurabh Malani***, *Ioannis G. Kevrekidis*
2:24 Paper 303g: Performance-Oriented Learning of Hybrid Models for Model Predictive Control — ***Georgios Makrygiorgos***, *Angelo D. Bonzanini, Victor Miller, Ali Mesbah*
2:43 Paper 303h: Learning-Based Economic Model Predictive Control for Energy Storage Systems Under Imperfect Forecast Information — ***David Pérez-Piñeiro***, *Sigurd Skogestad*

(304) Design and Analysis of Carbon Capture and Negative Emissions Technologies - Experimental

Tuesday, Nov 9, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 309

Dora Lopez De Alonzo, Chair
Omar Guerra, Co-Chair

Sponsored by: Climate Change

12:30 Paper 304a: Development of a Low-Cost Non-Amine Sorbent-Based Technology for Direct Air Capture of CO_2 — ***Cory Sanderson***, *Arnold Toppo, Raghubir Gupta*
12:45 Paper 304b: Experimental Characterization of Sorbents for Direct Air Capture of Carbon Dioxide — ***Thiago Stangherlin Barbosa***, *Klaus S. Lackner, John F. Cirucci, Matthew D. Green*
1:00 Paper 304c: Coupling Accelerated Mineral Carbonation and Direct Air Capture Processes — ***Raghavendra Ragipani***, *Keerthana Sreenivasan, Bu Wang*
1:15 Paper 304d: Flexible Low Temperature CO_2 Capture System, E-Cachys™— *Aaron Koenig, Teagan Nelson,* ***Srivats Srinivasachar***, *Junior Nasah, Johannes van der Watt*

(305) Design, Engineering, and Structural Prediction of Peptides and Proteins

Tuesday, Nov 9, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 108

Devleena Samanta, Co-Chair
Cemal Erdem, Co-Chair
Phanourios Tamamis, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

12:30 Paper 305a: Design of High Affinity, Specificity, and Stability Pro-Apoptotic Stapled Peptides Using Bacterial Cell Surface Display — ***Marshall Case***, *Greg Thurber*
12:48 Paper 305b: Engineering Latency-Associated Peptide for Potent TGF-β Inhibition — ***Lawrence A. Stern***
1:06 Paper 305c: RGN2- Single-Sequence Protein Structure Prediction with Applications in Protein Design and Novel Biomaterials — ***Ratul Chowdhury***
1:24 Paper 305d: Computationally-Designed 10th Type III Fibronectin Domains for Peptide Binding — ***Ritankar Bhattacharya***, *Varun Chauhan, Robert Pantazes*
1:42 Paper 305e: Engineering CRISPR-Cas9 with Relaxed PAM Specificity for Gene Repression — ***Yuxi Teng***, *Jian Wang, Ruihua Zhang, Yusong Zou, Yifei Wu, Yajun Yan*
2:00 Paper 305f: The Identity of Cargo Charge and Length Affect Cell Penetrating Peptide Mediated Cellular Internalization — ***Alireza Rahnama***, *Hannah C. Hymel, Olivia Sanchez, Ted J. Gauthier, Adam Melvin*
2:18 Paper 305g: High-Throughput Molecular Simulations and Experiments for Machine Learning Guided Protein Engineering (Invited Speaker) — ***Diwakar Shukla***

(306) Division Plenary: Valorization of Waste plastics including Ocean Plastics along with Agro-residues/Forestry waste for Sustainable Biocomposites (Invited Talks)

Friday, Nov 19, 8:00 AM
Virtual, Forest and Plant Bioproducts Division (17)

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

Sponsored by: Forest and Plant Bioproducts Division

8:00 Paper 306a: Properties and Applications of Biofoam Composite Materials— ***Gregory M. Glenn***
8:30 Paper 306b: Sustainable Plastics at NRC: Towards Zero Plastic Waste and Circular Economy — ***Karen Stoeffler***, *Damien Maillard*
9:00 Paper 306c: On Utilization of Agrowastes for Biocomposites and Biochar— ***Veera Boddu***
9:30 Paper 306e: Circular tools, materials and business models for a circular economy — ***Matthew Smyth***
10:00 Paper 306d: Waste Valorization and Sustainable Biocomposites Towards a Circular Economy: Current Status and Future Opportunities — ***Manjusri Misra***

(307) Electrochemical Fundamentals: Faculty Candidate Session I

Tuesday, Nov 9, 12:30 PM
Sheraton Back Bay, Commonwealth

Matthew Gebbie, Chair
Wenzhen Li, Co-Chair

Sponsored by: Electrochemical Fundamentals

12:30 Paper 307a: Effects of Temporal Parameters of Pulsed Electric Field Operation on Desalination Performance and Water Dissociation in Electrodialysis — ***Soraya Honarparvar***, *Rashed Al-Rashed, Amos Winter*
12:50 Paper 307b: Catalyst Synthesis for Fuel Cell Application and Fundamental Understanding of CO_2 Reduction Mechanism — ***Bjorn Hasa***
1:10 Paper 307c: Comparison of Thermal- and Electro-Catalytic Conversion of Biomass-Derived Oxygenates — ***Reda Bababrik***, *Bin Wang, Daniel E. Resasco*
1:30 Paper 307d: Understanding the Extent of Ionic Dissociation and Ionic Conductivity in Model Thin Film Polymer Electrolytes As a Function of Different Side Chain Configurations — ***Mario Ramos-Garces***, *Ishara Senadheera, Revati Kumar, Christopher Arges*
1:50 Paper 307e: Elucidating the Functionality of Hydroxide Electrolyte in Anion-Exchange-Membrane Water Electrolyzer — ***Jiangjin Liu***, *Dongguo Li, Shaun Alia, Cy Fujimoto, Adam Weber*
2:10 Paper 307f: Relationship between Aerobic Oxidation Catalysis and Electrochemical O_2 Reduction on Heterogeneous M–N–C Catalysts — ***Jason S. Bates***, *Sourav Biswas, Sung-Eun Suh, Biswajit Mondal, Mathew R. Johnson, Spencer M. Runde, Thatcher W. Root, Shannon S. Stahl*
2:30 Paper 307g: Electrochemical Reactions: Fundamentals Mapped from the Atomic to the Macroscopic Scale — ***Joakim Halldin Stenlid, PhD***

(308) Enabling Technologies Relevant to Drug Substance and Drug Product II

Tuesday, Nov 9, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 102

David Am Ende, Chair
Dana Barrasso, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

12:30: Break
12:54 Paper 249d: A Novel Technology for Continuous Vacuum Drying of an API Slurry: Characterization of Product — ***Isabella Aigner***, *Manuel Zettl, Peter van der Wel, Hartmuth Schröttner, Markus Krumme, Johannes G. Khinast*
1:18 Paper 308b: Use of Bead Mixtures As an Enabling Approach for Optimal Production of Drug Nanosuspensions — ***Gulenay Guner***, *Manisha Kannan, Matthew Berrios, Ecevit Bilgili*
1:42 Paper 308d: A Robust Micro-Dosing Approach for Pharmaceutical Powders Based on a Small-Scale Powder Pump Concept — ***Andreas Kottlan***, *Jakob Geistlinger, Benjamin Glasser, Johannes G. Khinast*
2:06 Paper 372d: Pharmaceutical HME Process Development: Understanding the Impact of Kneading Elements in the Screw Configuration and Product Quality — ***Josip Matic***, *Hannes Bauer, Rachel C. Evans, Andreas Gryczke, William Ketterhagen, Kushal Sinha, Johannes G. Khinast*
2:30 Paper 308e: Continuous Low Dose Powder Feeder — *Johannes G. Khinast, Stephan Sacher,* ***Sara Fathollahi***

(309) Feedstock Conversion Interface Consortium – Understanding Feedstock Variability to Enable Next Generation Biorefineries II (Invited Talks)

Monday, Nov 15, 3:30 PM
Virtual, Sustainable Engineering Forum (23)

Vicki Thompson, Chair
Edward Wolfrum, Co-Chair

Sponsored by: Sustainable Biorefineries

3:30: Introductory Remarks
3:40 Paper 309a: Recent Progress on the Development of a Virtual Feedstock Preprocessing & Handling Laboratory — ***Yidong Xia***, *Wencheng Jin, Jordan Klinger, Tiasha Bhattacharjee, Vicki Thompson*
4:05 Paper 309b: Modelling a Compressible Packed Bed Flow-through Deacetylation Reactor for Corn Stover Pretreatment — ***Yudong Li***, *Xiaowen Chen, David A. Sievers*
4:30 Paper 309c: Multi-Scale Fast Pyrolysis Simulation Framework for Varied Biomass Feedstocks — ***Liqiang LU***, *Xi Gao, Mehrdad Shahnam, William Rogers*
4:55 Paper 309d: Technoeconomic and Sustainability Impacts of Feedstock Variability and Mitigation within the Biomass-to-Fuels Value Chains for Corn Stover and Forest Residues — ***Steven Phillips***, *Erin Webb*
5:20 Paper 309e: TEA Modeling to Quantify Economic Implications for Biorefinery Processing of Isolated Anatomical Fractions of Corn Stover — ***Ryan Davis***, *Ian McNamara, Andrew Bartling*
5:45 Paper 309f: Dynamic Life-Cycle Analysis of Fast Pyrolysis Conversion: Implications on Strategies to Manage Feedstock Variability and Improve Sustainability — ***Hao Cai***, *Longwen Ou*

(310) Fuel Processing for Hydrogen Production

Tuesday, Nov 9, 12:30 PM
Marriott Copley Place, Fairfield

Dushyant Shekhawat, Chair
Daniel J. Haynes, Co-Chair
Jianli Hu, Co-Chair

Sponsored by: Fuels and Petrochemicals Division

12:30 Paper 310b: Catalytic CO2 Conversion in Relevant Industrial Environments. a Steel Mill Case — *Juan Carlos Navarro, Miguel A. Centeno, Oscar Laguna, **José A. Odriozola***
12:50 Paper 555d: Natural Gas Pyrolysis: Advantaged Production of Low-Emissions Hydrogen and Carbon Materials — *David Dankworth, Jayashree Kalyanaraman, A. Sarma Kovvali, Sophie Liu, Ying Liu, **Steven Pyl**, Sumathy Raman, Ramon Strauss, Joshua Willis*
1:10 Paper 310d: Cellulose As a New Templating Agent for Combustion Synthesis of NiO-MgO Solid Solution Catalysts for the Dry Reforming of Methane — ***Vardan Danghyan**, Alexander Mukasyan, Eduardo E. Wolf*
1:30 Paper 310e: A Novel Photocatalytic Process for Electrification of Hydrogen Production By Steam Methane Reforming. — ***Syed Gardezi***
1:50 Paper 310f: Photobacteria-Based Biohydrogen Production from Organic Waste By the Use of Near-IR Light and Plasmonic Nanoparticles — ***Dibakar Bhattacharyya**, Noah D. Meeks, Doo Young Kim, J. Todd Hastings, Yuxia Ji*

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

Tuesday, Nov 9, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 310

Anita Shukla, Chair
Angela Brown, Co-Chair

Sponsored by: Microbes at Biomedical Interfaces

12:30 Paper 311a: Microbial Growth and Microbial Community Assembly in Household Water Pipes — ***Fangqiong Ling***
1:00 Paper 311b: Fighting Bacteria: A Computational Exploration of Bacterial Interactions — ***Kimberly Bowal**, Brian Analikwu, Timon Idema*
1:30 Paper 311c: Biofilm Growth Morphology in Confined Heterogenous Media— ***R. Konane Bay**, Sujit Datta*
2:00 Paper 311d: Deconvolute Bacterial Responses to Surface Nanotopography and Surface Chemistry Using Orthogonally Engineered Biointerfaces — ***Yifan Cheng**, Rong Yang*
2:30 Paper 311e: Molecular Dynamics Investigation of Biomolecule Adsorption to Graphene and Modified Graphene: Molecular Insights into Biofilm Formation and Adhesion — ***Sourav Verma**, Kenneth Benjamin*

(312) Fundamental Research in Transport Processes

Tuesday, Nov 9, 12:30 PM
Sheraton Back Bay, Republic Ballroom A

Joel Plawsky, Chair
Samaneh Farokhirad, Co-Chair

Sponsored by: Transport Processes

12:30 Paper 312a: Controlled Release of Molecular Intercalants in Graphene Oxide Films: Edge and Basal-Plane-Specific Kinetics of Planar, 1D Wrinkled, and 2D Crumpled Nanochannels — *Muchun Liu, **Deisy Cristina Carvalho Fernandes**, Zachary Saleeba, Robert Hurt*
12:45 Paper 312b: Multicomponent Diffusion of Interacting, Nonionic Micelles with Hydrophobic Solutes — ***Nathan Alexander**, Ronald J. Phillips, Stephanie R. Dungan*
1:00 Paper 312c: Early-Time Dynamics of Fluid-Driven Cracks — ***Pankaj Rohilla**, Idera Lawal, Noah Williams, Jeremy Marston*
1:15: Break
1:30: Break
1:45 Paper 312f: Understanding the Mechanisms of Liquid Dynamics — ***Kelly Badilla**, Marcus T Cicerone, Andreas Bommarius*
2:00 Paper 312g: Velocity Distribution for Flow in Porous Media — ***Vi Nguyen**, Dimitrios Papavassiliou*
2:15 Paper 312h: Internal Hydraulic Jump Induced Slugging and Flooding in Two Phase Gas-Liquid Flow — *Mrinmoy Dhar, Subhabrata Ray, **Gargi Das**, Prasanta Kumar Das*
2:30 Paper 312i: Plug Generation Mechanisms and Reaction Rates for Liquid-Liquid Flow Systems in Mesoscale — *Alex Koshy, **Gargi Das**, Subhabrata Ray*

(313) Highly Selective Separations with Membranes I

Tuesday, Nov 9, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 304

Dibakar Bhattacharyya, Co-Chair
Christine Duval, Co-Chair

Sponsored by: Membrane-Based Separations

12:30 Paper 682d: One-Step Desalination and Targeted Solute Capture Using Ion-Capture Electrodialysis — ***Adam Uliana**, Ngoc Bui, Jovan Kamcev, Mercedes Taylor, Jeffrey J. Urban, Jeffrey R. Long*
12:45 Paper 313b: Tuning Electrostatic Interactions for Selective Electrochemical Organic Acid Separations — ***Matthew Jordan**, Yupo Lin, Christopher Arges*
1:00 Paper 313c: Enhancing Selectivity through Fluorination — ***Zachary Smith**, Albert X. Wu*
1:15 Paper 313d: Graphene Oxide Composite Membranes with Locked Interlayer Nanostructure for Ethanol/Water Separation — ***Bratin Sengupta**, Dinesh Behera, Qiaobei Dong, Fanglei Zhou, Huazheng Li, Georges Belfort, Miao Yu*
1:30 Paper 313e: Analysis of the Transport of Guest Molecules in Molecularly Mixed Composite Membranes Containing Porous Organic Cages — ***Matthew Rivera**, Ryan Lively*
1:45 Paper 682b: Membrane Protein-Based Biomimetic Membranes for Water Treatment — ***Yu-Ming Tu**, Hyeonji Oh, Benny D. Freeman, Manish Kumar*
2:00 Paper 313g: Separating Liquid Mixture Using Supported Ionic Liquid Membranes (SILMs) — ***Aigerim Baimoldina**, Lei Li*

(314) Hydrocarbon Conversion: Catalytic Pathways

Tuesday, Nov 9, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 205

Yizhi Xiang, Chair
Lev Davydov, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

12:30 Paper 314a: Simultaneous Activation of CH_4 and N_2 in a Microwave Enhanced Plasma-Catalytic Hybrid Reactor — ***Sarojini Tiwari**, Brandon Robinson, Jianli Hu*
12:48 Paper 314b: Rationalizing Ethylene Oligomerization on Single Site Ga^{3+}Catalysts on Amorphous Silica: A First Principles Study Combined with Microkinetic Modeling and Experiments — ***Yinan Xu**, Nicole LiBretto, Jeffrey T. Miller, Jeffrey Greeley*
1:06 Paper 314c: Cu-Exchanged SSZ-13 in the Stepwise Conversion of Methane to Methanol — ***Florian Goeltl**, Saurabh Bhandari, Edgard Lebron Rodriguez, Jake Gold, Ive Hermans, Stacey Zones, James A. Dumesic, Manos Mavrikakis*
1:24 Paper 314e: Catalytic Diversity in MFI Zeolites for Brønsted Acid-Catalyzed Propene Oligomerization: Consequences of Crystallite Properties and Active Site Proximity — ***Elizabeth Bickel**, Lauren Kilburn, Claire Nimlos, Young Gul Hur, David Hibbitts, Rajamani Gounder*
1:42 Paper 314f: Ethylene Oligomerization on Ni/Uio-66: Rates, Mechanism, and Site Densities — ***Benjamin Yeh**, Stephen Vicchio, Saumil Chheda, Jian Zheng, Julian Schmid, Laura Löbbert, Ricardo Bermejo-Deval, Oliver Gutiérrez-Tinoco, Johannes A. Lercher, Connie C. Lu, Matthew Neurock, Rachel Getman, Laura Gagliardi, Aditya Bhan*
2:00 Paper 314g: Kinetic Modeling of Ethene Oligomerization over Bifunctional Ni-Exchanged Acid Zeolites — ***Elsa Koninckx**, Joris Thybaut, Linda Broadbelt*
2:18 Paper 314h: A Novel Route for Alkenes and Cycloalkanes Via Ethylene Oligomerization over Heterogeneous Ni-Siral Catalysts — ***Gabriel Viana Sueth Seufitelli**, Fernando Resende, Rick Gustafson*
2:36 Paper 673f: Ammonia Reforming of Ethane over Re Supported HZSM-5 Catalyst — ***Siavash Fadaeerayeni**, Genwei Chen, Hossein Toghiani, Yizhi Xiang*

(315) Hydrogel Biomaterials: Design and Characterization

Tuesday, Nov 9, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 105

Murat Guvendiren, Chair
Marjan Rafat, Co-Chair
Adam Ekenseair, Co-Chair
Amir Sheikhi, Co-Chair

Sponsored by: Biomaterials

12:30 Paper 315a: 3D Bioprinting of Dynamic Covalent Hydrogels Using a Small Molecule Competitor and Catalyst — ***Sarah Hull**, Christopher D. Lindsay, Junzhe Lou, Ashley Westerfield, Lucia G. Brunel, Yan Xia, Sarah C. Heilshorn*
12:48 Paper 315b: Enhanced Granular Hydrogel Properties through Dynamic Covalent Interparticle Crosslinking — ***Victoria Muir**, Jason A. Burdick*
1:06 Paper 315c: Control of Biocompatible Hydrogel Mechanics with Polymer Persistence Length — ***Logan Morton**, Adrianne Rosales*
1:24 Paper 315d: Double Network Hydrogel Bioadhesives with Tunable Adhesive and Cohesive Properties — ***Defu LI**, Shima Gholizadeh, Mahsa Ghovvati, Nasim Annabi, Samanvaya Srivastava*
1:42 Paper 315e: Microstructure-Property Correlation in Hybrid Colloidal Gels Based on Gelatin Nanoparticles and Silicate Nanoplatelets — ***Gelareh Rezvan**, Mohsen Esmaeili, Monirosadat Sadati, Nader Taheri-Qazvini*
2:00 Paper 315f: Integration of Calcium Responsiveness into Self-Healing Protein Hydrogels through Consensus Repeat Sequence Engineering — *Marina P. Chang, **Danielle Mai***
2:18 Paper 315g: Investigating the Network Structure and Transport Properties of Physically Crosslinked Lignin-Based Composites — ***Keturah Bethel**, Graham Tindall, Madeline McCarthy, Mark Thies, Eric M. Davis*
2:36 Paper 315h: Solid-State NMR Molecular Structural Analysis of Co-Assembled Peptide Nanofibers. — ***Anant Paravastu***

(316) In Honor of Johannes Schwank's 70th Birthday (Invited Talks)

Tuesday, Nov 9, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 210

Abhaya Datye, Chair
Levi T. Thompson, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

12:30: Introductory Remarks
12:31 Paper 316a: Single Atom Catalysis: From an Academic Curiosity to Industrial Applications — ***Abhaya K. Datye***
12:49 Paper 316b: Impact of Precious Metal Supply and Demand on the Technology Choices for Three-Way Catalysts — ***Galen Fisher***
1:07 Paper 316c: The Curious Redox Behavior of Supported Pd – a Review of Current Understanding — ***Robert McCabe***

1:25 Paper 316d: From Surface Science to Powder Catalysis: Underlying Mechanistic Insights — ***Manos Mavrikakis***
1:43 Paper 316e: Recent Progress on Ni-Based Cermet Anodes for Intermediate-Temperature Solid Oxide Fuel Cells — *Tian Gan, Yicheng Zhao,* ***Yongdan Li***
2:01 Paper 316f: Oxygen Reduction Reaction on Pt Electrodes: From Kinetics and Spectroscopy to New Materials — ***Suljo Linic***
2:19 Paper 316g: Controlling Discharge Product Distribution through an Electrode Surface-Mediated Mechanism in Alkali Metal-O_2 Battery Cathodes— ***Eranda Nikolla***
2:37 Paper 316h: Using Cascade Concepts to Design More Energy and Atom Efficient Heterogeneous Catalysts — ***Levi T. Thompson***
2:55: Concluding remarks by Prof. Johannes Schwank

(317) Integrated Product and Process Design

Tuesday, Nov 9, 12:30 PM
Sheraton Back Bay, Back Bay Ballroom C

Alexander Dowling, Co-Chair
Ana I. Torres, Co-Chair

Sponsored by: Systems and Process Design

12:30 Paper 317a: Biorefinery Synthesis-a Route Towards Engineered Advanced Fuels — ***Juan Manuel Restrepo-Florez****, Joonjae Ryu, David Rothamer, Christos Maravelias*
12:51 Paper 317b: Molecular Design Targets and Optimization of Low-Temperature Thermal Desalination Systems — ***Alejandro Garciadiego****, Tengfei Luo, Alexander Dowling*
1:12 Paper 317c: Energy Integration through Retrofitting of Heat Exchanger Network at Equinor Kalundborg Oil Refinery — ***Niels Sørensen****, Lars Erik Ebbesen, Haoshui Yu, Gürkan Sin, Jesper Vester Leihof Nielsen*
1:33 Paper 317d: Simultaneous Synthesis of Metabolic and Process Engineering for the Production of Muconic Acid — *Konstantinos Dimitriou,* ***Antonios Kokosis***
1:54 Paper 317e: Process Design for the Production of Xylitol in a Multi-Product Biorefinery — ***Nikolaus Vollmer****, Krist V. Gernaey, Gürkan Sin*
2:15 Paper 317f: Digital Design of a Lomustine Manufacturing Process Using Pharmapy — ***Daniel Casas-Orozco****, Daniel Laky, Inyoung Hur, Jaron Mackey, Ahmed Mufti, Gintaras V. Reklaitis, Zoltan Nagy*
2:36 Paper 317g: SPICE_ED: A Framework for Simultaneous Materials Screening and Process Synthesis for Extractive Distillation — ***Mohammed Sadaf Monjur****, Ashfaq Iftakher, M M Faruque Hasan*

(318) Interfacial and Nonlinear Flows

Tuesday, Nov 9, 12:30 PM
Sheraton Back Bay, Constitution B

Satish Kumar, Co-Chair
Ankur Gupta, Co-Chair

Sponsored by: Fluid Mechanics

12:30 Paper 318a: Modeling and Simulation of Hydrogel Interfacial Dynamics— ***Pengtao Yue****, Lei Li, Jiaqi Zhang, Zelai Xu, Yuan-Nan Young, James J. Feng*
12:45 Paper 318b: Bifurcation Pattern Formation in Biological Tissues: A New Discovery of Interfacial Instability with Applications in Healthcare — ***Amir Hejri****, John M. Nickerson, Mark R. Prausnitz*
1:00 Paper 318c: Rayleigh-Taylor Waves in Viscoelastic Fluids- an Unintuitive Result — ***Naga Venkata Satya Siva Rama Dinesh Bhagavatula****, Ranga Narayanan*
1:15 Paper 318d: Effects of Elasticity on Fingering Instabilities — ***Fahed Albreiki****, Alexander Kubinski, Prerana Rathore, Andrew Rasmussen, Vivek Sharma*
1:30: Break
1:45 Paper 318f: Understanding Interfacial Interactions in Bijels — ***Douglas Tree****, Rami Alhasan*
2:00 Paper 318g: Non-Axisymmetric, Dynamic Evolution of Thin Liquid Films over Curved Substrates — *Eric Shaqfeh,* ***Xingyi Shi****, Gerald Fuller, Mariana Rodriguez-Hakim, Theo Yang*
2:15 Paper 318h: Capillary-Flow Dynamics in Open Rectangular Microchannels— *Panayiotis Kolliopoulos, Krystopher S. Jochem, Danirel Johnson, Wieslaw J. Suszynski, Lorraine F. Francis,* ***Satish Kumar***
2:30 Paper 318i: The Effect of Gravity on the Shape of a Droplet on a Fiber in the Limit of Small Bond Numbers: Nearly Axisymmetric Profiles with Experimental Validation — ***Ankur Gupta****, Andrew Konicek, Mark King, Azmaine Iqtidar, Mohsen Yeganeh, Howard A. Stone*
2:45 Paper 318j: Transport Limits on Dissolution from a Rotating Disk –Effects of Instabilities in the Flow — ***Ziyao Liu****, Tony Ladd*

(319) Interfacial Phenomena in Pharmaceutics

Tuesday, Nov 9, 12:30 PM
Sheraton Back Bay, Back Bay Ballroom B

Prajnaparamita Dhar, Chair
Mark Kastantin, Co-Chair

Sponsored by: Interfacial Phenomena

12:30 Paper 319a: Quantifying the Effects of Recombinant Human Lubricin on Model Tear Film Stability — ***Kiara Cui****, Vincent Xia, Daniel Cirera Salinas, David Myung, Gerald Fuller*
12:45 Paper 319c: Interfacial Rheology of Monoclonal Antibodies — ***Eric Furst****, Caitlin Wood, Christopher Roberts, Jan Vermant*
1:00 Paper 319d: Characterizing Self-Association and Clustering in Antibody Solutions at High Concentrations Using x-Ray Scattering, Rheology and Coarse Grained Simulation — ***Neha Manohar****, Amjad Chowdhury, Thomas Truskett, Keith Johnston*
1:15 Paper 319e: Volume and Frequency Selective NMR Spectroscopy of Monoclonal Antibodies at Water-Oil Interfaces — *Jamini Bhagu, Samuel C. Grant,* ***Hadi Mohammadigoushki***
1:30 Paper 319g: Quantifying Effects of Polar Lipid Proportions on Model Tear Film Stability — ***Vincent Xia****, Kiara Cui, David Myung, Gerald Fuller*
1:45 Paper 319h: Influence of Salt on the Separation Mechanics on Droplet Interface Phospholipid Bilayers — ***Yaoqi Huang****, Vineeth Chandran Suja, Layaa Amirthalingam, Gerald Fuller*
2:00 Paper 319i: Inactivation of Lung Surfactant By Phospholipase-Catalyzed Degradation — ***Julia Fisher****, Todd Squires*
2:15 Paper 319j: Cholesterol Induced Morphological Instabilities and Transitions in Phospholipid Monolayers — ***Cain Valtierrez-Gaytan****, Joseph Barakat, Benjamin Stottrup,* ***Joseph Zasadzinski***

(320) LGBTQ+ & Allies Safe Zone Workshop

Tuesday, Nov 9, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 204

Anthony Butterfield, Chair
Alon McCormick, Co-Chair

Sponsored by: LGBTQ+ and Allies Community

(321) Materials for Electronics, Lighting, and Light-Matter Interactions

Tuesday, Nov 9, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 104

Andrej Lenert, Chair
Shikai Deng, Co-Chair

Sponsored by: Electronics and Photonics

12:30 Paper 321a: Iron-Tunable, Visible-Frequency Optical Resonances in Colloidal Intermediate-Band Semiconductor Nanocrystals — *Soohyung Lee, Sandeep Ghosh, Chad Hoyer, Hongbin Liu, Xiaosong Li,* ***Vincent Holmberg***
1:00 Paper 321b: Structure, Stability, and Optoelectronic Properties of Silicon Nanomaterials — ***Matthew Panthani***
1:15 Paper 321c: Dielectric Nanostructures for Solar Light Harvesting Applications — ***Sundaram Bhardwaj Ramakrishnan****, Ravi Teja Addanki Tirumala, Farshid Mohammadparast, Marimuthu Andiappan*
1:30 Paper 321d: Direct Detection of Optical Resonance Modes in Meta-Atoms Fabricated By Metallization of DNA Origami Templates — ***Md Monirul Islam****, Md Mir Hossen, Pierre E Palo, Lee Bendickson, Marit Nilsen-Hamilton, Thomas Koschny, Andrew C. Hillier*
1:45 Paper 321e: Controlling Structure-Property Relationships of Organic Semiconductor Thin Films Using Tunable, Highly-Ordered Self-Assembled Monolayers — ***Ashley Conley****, Gaurav Giri, Joshua Choi*
2:00 Paper 321f: Using Metal Nanocrystal Photothermal Heating to Drive Colloidal Semiconductor Nanowire Growth — ***Matthew Crane****, Elena P. Pandres, E. James Davis, Peter Pauzauskie, Vincent Holmberg*
2:15 Paper 321g: Electric-Field Induced Luminescence Shift for Excited States at Organic Semiconductor Interfaces — ***Nolan Concannon****, Russell J. Holmes*

(322) Mind the Gap: Industrial Perspectives on Educating Chemical Engineers (Invited Talks / Panel Discussion)

Tuesday, Nov 9, 12:30 PM
Sheraton Back Bay, Republic Ballroom B

Daniel Lepek, Chair
Matthew Liberatore, Co-Chair

Sponsored by: Education

(323) New Developments in Computational Catalysis II: Active Sites in Complex Materials

Tuesday, Nov 9, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 206

Matthew Montemore, Chair
G. T. Kasun Kalhara Gunasooriya, Co-Chair
Alexander Mironenko, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

12:30: Break
12:50 Paper 323b: Grafting $TiCl_4$ Onto Amorphous Silica: Modeling Effects of Silanol Heterogeneity — ***Salman Khan****, Craig Vandervelden, Sahan Godahewa, Pubudu N. Wimalasiri, Ward H. Thompson, Susannah L. Scott, Baron Peters*
1:10 Paper 323c: Probing Shape-Selective Catalysis in Heterogeneous Nanoporous Catalysts — ***Shubham Malviya****, Peng Bai*
1:30 Paper 323d: Towards the Design of Active Site Requirements for the Selective Hydrogenation of Different Functionalities — ***Angela Nguyen****, Unnatti Sharma, Michael J. Janik, Zachary Ulissi*
1:50: Break
2:10 Paper 323f: Bayesian Analysis for Identifying the Active Sites for Platinum Catalyzed Propane Dehydrogenation: Bridging Experiments, Density Functional Theory, and Reactor Modeling. — ***Charles Fricke****, Andreas Heyden*
2:30 Paper 323g: Role of Metastable Active Sites in C-H Bond Activation of C1 and C2 Molecules — ***Sonit Balyan****, Shikha Saini, Tuhin Suvra Khan, K. K. Pant, Puneet Gupta, Saswata Bhattacharya, M. Ali Haider*

(324) Novel Reactors I (Targeted/Localized Heating Strategies)

Tuesday, Nov 9, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 300

Robert Broekhuis, Chair
Kishori Deshpande, Co-Chair

Sponsored by: Process Intensification & Microprocess Engineering

12:30 Paper 324a: Electromagnetic Simulations Aided Stable Microwave Reactor Configuration — ***Abhinav Malhotra***, *Weiqi Chen, Weiqing Zheng, Pedro Plaza-Gonzalez, Jose M. Catala-Civera, Jesus Santamaria, Dionisios Vlachos*
12:55 Paper 324b: Decoupling MW Sensitivity and Reactivity: Towards Understanding Fe-ZSM-5@SiC As Effective Microwave Catalyst for Methane Dehydro-Aromatization — ***Sanjana Karpe***, *Xinwei Bai, Jianli Hu, Goetz Veser*
1:20 Paper 324c: Controlling Homogeneous/Heterogeneous Reactions in Alkane Dehydrogenation — ***Weiqi Chen***, *Kewei Yu, Abhinav Malhotra, Weiqing Zheng, Pedro Plaza-Gonzalez, Jose M. Catala-Civera, Raul Lobo, Dionisios Vlachos*
1:45 Paper 324d: Microwave Heating of Liquid-Liquid Biphasic Systems— ***Montgomery Baker-Fales***, *Tai-Ying Chen, Himanshu Goyal, Dionisios Vlachos*
2:10 Paper 324e: Microwave Fluidized Bed and Microwave Hybrid Fixed Bed Reactor for the Ethane Dehydroaromatization Reaction — ***Brandon Robinson***, *Ashley Caiola, Jianli Hu*

(325) Particle Breakage and Comminution Processes

Tuesday, Nov 9, 12:30 PM
Sheraton Back Bay, Fairfax A/B

Sheena Reeves, Chair
Sarang Oka, Co-Chair
Jung-Sheng Wu, Co-Chair

Sponsored by: Particle Production and Characterization

12:30 Paper 325a: Discrete Element Method Analysis for the Mechanochemical Grinding of Polymers — ***William Bradley***, *Elisavet Anglou, Andrew Tricker, Carsten Sievers, Fani Boukouvala*
12:55 Paper 325b: Effect of Aspect Ratio on Breakage Kinetics of Urea Crystals in Agitated Slurries — ***Priscilla Hill***
1:20 Paper 325c: Simulation of Full-Scale Open-Circuit, Multi-Compartment Cement Ball Mills: A New True Unsteady-State Simulator — *Nontawat Muanpaopong,* ***Rajesh Dave***, *Ecevit Bilgili*
2:10 Paper 325e: Milling Studies in an Impact Crusher I: Population Balance Modelling and the Effect of Speed and Particle Size on Particle Size Distribution— ***Ngonidzashe Chimwani***, *Murray Bwalya*

(326) Particulate and Multiphase Flows: Colloids and Polymers

Tuesday, Nov 9, 12:30 PM
Sheraton Back Bay, Constitution A

Melissa Gordon, Chair
Henry Chu, Co-Chair

Sponsored by: Fluid Mechanics

12:30 Paper 326j: Linear Viscoelastic Properties of Adhesive Soft Particle Glasses — *Ali Shahmohammadi,* ***Roger Bonnecaze***
12:45 Paper 326a: Rheological Properties of Phase Transitions in Polydisperse and Monodisperse Colloidal Rod Systems — ***Shiqin He***, *Dominic Pascucci, Marco Caggioni, Seth Lindberg, Kelly Schultz*
1:00 Paper 326b: Time-Varying Flows of Concentrated Suspensions of Rigid Fibers — ***Jason Butler***, *Scott Strednak, Elisabeth Guazzelli, Laurence Bergougnoux*
1:15 Paper 326c: A Multiscale Tensorial Approach for Modeling the Rheology of Thixotropic Aggregating Suspensions — ***Soham Jariwala***, *Norman J. Wagner, Antony Beris*
1:30 Paper 326d: Experiments and Numerical Simulations of the Shear Rheology of Particulate Suspensions in Shear-Thinning Elastic Fluids — ***Anni Zhang***, *Eric Shaqfeh*
1:45 Paper 326e: Rheological Modeling of Living Polymers: Practical Tools for Systems That Are Not 'fast Breaking' — ***Joseph Peterson***, *Michael Cates*
2:00 Paper 326f: Modeling of the Time-Dependent Rheological Behavior of Particulate Suspensions — ***Babajide Onanuga***, *Abdul Salam Mohammad, Joseph J. Biernacki*
2:15 Paper 326g: Flow and Microstructure of Colloidal Gels with Telechelic Polymers — ***Kristine M. Smith***, *Lilian Hsiao*
2:30 Paper 326h: Temperature-Induced Aggregation and Rheological Response of Concentrated Portlandite Suspensions — ***Sharu Bhagavathi Kandy***, *Iman Mehdipour, Narayanan Neithalath, Mathieu Bauchy, Edward Garboczi, Torben Gädt, Samanvaya Srivastava, Gaurav Sant*
2:45 Paper 326i: Crystalline Shielding Localizes Memory in Jammed Systems Under Oscillatory Shear — ***Erin Teich***, *K. Lawrence Galloway, Paulo E. Arratia, Danielle S. Bassett*

(327) Polymer Thin Films, Confinement, and Interfaces I

Monday, Nov 8, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 101

Stephen Martin, Chair
Rong Yang, Co-Chair
Kathleen McEnnis, Co-Chair
Caroline Szczepanski, Co-Chair

Sponsored by: Polymers

12:30 Paper 327a: Pseudoentanglements Produce Rubbery Surface atop Polymer Glasses — ***Rodney Priestley***
1:00 Paper 327b: Designing Complex Polymer Colloids for Films with Enhanced Properties and Self-Stratification — ***Piyush Singh***, *Michaeleen Pacholski, Junsi Gu, Luke Yu, Yookyung Go, Cecilia Leal, Kshitish Patankar, Ray Drumright, Simon Rogers, Charles M. Schroeder*
1:15 Paper 327c: Selection and Processing of Food Grade Plasticizers to Compatibilize Cellulose Nanocrystals / Ethylene Vinyl Alcohol Copolymer Nanocomposites — *Md Nuruddin, Justin Hamlin, Caitlyn Clarkson, John Howarter,* ***Caroline Szczepanski***, *Jeffrey Youngblood*
1:30 Paper 327d: Influence of Polymer Diffusivity in Nanoconfinement on the Onset of Viscous Fingering — *Thitiporn Kaewpetch, Samuel Wilson-Whitford, Christian Heil, Arthi Jayaraman,* ***James Gilchrist***
1:45 Paper 327e: Patterning Shape Memory Polymer Photonic Crystal Membranes through Supplemental UV Exposure — ***Calen Leverant***, *Yifan Zhang, Peng Jiang*
2:00 Paper 327f: Direct Quantification of Polymer Chain Dimensions Using End-to-End Förster Resonance Energy Transfer — *Alexander Fortenberry,* ***Zhe Qiang***
2:15 Paper 327h: Morphology Transitions in Lamellar Block Copolymer Thin Films between Direct Solvent Immersion Annealing and Thermal Annealing— ***Kshitij Sharma***, *Ali Masud, Guangcui Yuan, Sushil Satija, Jack F. Douglas, Alamgir Karim*
2:30 Paper 327i: Comparison of Long-Term Stability of Initiating Monolayers in Surface-Initiated Controlled Radical Polymerizations — ***Mingxiao Li***, *Michele Fromel, Dhanesh Ranaweera, Christian Pester*
2:45 Paper 694f: Super-Hydrophilic Anti-Fogging Coatings Via Aqueous Surface-Initiated Photopolymerization — ***Michele Fromel***, *Devon Sweeder, Christian Pester*

(328) Powder and Particulate Characterization and Measurement: In-person

Tuesday, Nov 9, 12:30 PM
Sheraton Back Bay, Gardner

Richard Lueptow, Chair
Shankali Pradhan, Co-Chair

Sponsored by: Solids Flow, Handling and Processing

12:30 Paper 328a: Characterization of Polymeric Powders through Capillary Flow for Additive-Manufacturing Techniques — ***Sebnem Ozbek***, *Katrina J. Donovan, Travis W. Walker*
12:45: Break
1:00 Paper 328f: Estimating the Three Characteristic Lengths of Plate-like Particles in Suspension — ***Pietro Binel***, *Ankit Jain, Anna Jaeggi, Daniel Biri, Ashwin Kumar Rajagopalan, Andrew J. deMello, Marco Mazzotti*
1:15 Paper 267c: Predicting the Behavior of Different Tablet Press Feed Frame Systems Using the Discrete Element Method (DEM) Modeling — *Zihao Li,* ***Rohit Kumar***, *Hector Guzman*
1:30: Break
1:45 Paper 267d: Fundamental Investigation of the Rheology and Structure of Capillary Suspensions Made with Oyster Particles — ***Pablo Garcia-Trinanes***, *Makrina A. Chairopoulou, Ulrich Teipel*

(329) Reaction Chemistry and Engineering I

Tuesday, Nov 9, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 207

Milad Abolhasani, Chair
Joshua Allen, Co-Chair
Pranit S. Metkar, Co-Chair
Andrew R Teixeira, Co-Chair
Pranav Karanjkar, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

12:30 Paper 329a: 3D-Printed Dual Functional Adsorbent Catalyst Monoliths for Combined CO_2 Capture and Ethane Dehydrogenation — ***Ali Rownaghi***,***Fateme Rezaei***, ***Kyle Newport***, *Shane Lawson, Daniel Hanify*
12:48 Paper 329b: Secondary Effectiveness Factors for Catalytic Reactions in Series: A Unified Extension to Slab, Cylinder, and Spherical Geometries— ***Armin Shayesteh Zadeh***, *Baron Peters*
1:06 Paper 329c: High-Performance Bifunctional Sulfur Carriers for Hydrogen Production from Hydrogen Sulfide with Regeneration Using Carbon Dioxide in Cyclic Redox Scheme — ***Kalyani Jangam***, *Anuj Joshi, Yu-Yen Chen, Shailaja Mahalingam, Ashin Antony Sunny, L.-S. Fan*
1:24 Paper 329d: Do Axial Thermowells Measure the True Temperature for Highly Exothermic Reactions in Fixed Beds? a CFD Analysis for Phthalic Anhydride Synthesis. — ***Anthony Dixon***, *Yan Wu*
1:42 Paper 329e: Automated Screening of Catalytic Reaction Mechanisms: A Tool for Novel Chemistries — ***Pedro Mendes***, *Vasco Saltão, Filipe G Freire, Laura Pirro, Joris Thybaut*

(330) Recent Advances in Multiscale Methodologies

Tuesday, Nov 9, 12:30 PM
Marriott Copley Place, Salon J/K

Nathan Mahynski, Chair
Kayla Sprenger, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

12:30 Paper 330a: Developing Multiscale Models of the Blood-Brain Barrier Interface for the Treatment of Alzheimer's Disease — ***Shikha Nangia***, *Nandhini Rajagopal*
12:43 Paper 330b: Exploring Non-Biological Foldamer Secondary Structure Using Tuneable Coarse-Grained Models — ***Theodore Fobe***, *Christopher Walker, Michael Shirts*
12:56 Paper 330c: [Invited Talk] Improving Accuracy of Systematic Coarse-Grained Simulations — ***Andrew White***
1:19 Paper 330d: A Multiscale Approach to Analyzing the Van Hove Correlations of Water — *Ray Matsumoto, Matthew W. Thompson, Van Quan Vuong, Weiwei Zhang, Yuya Shinohara, Adri C.T van Duin, Stephan Irle, Paul R.C. Kent, Takeshi Egami,* ***Peter Cummings***
1:32 Paper 330e: Revealing Mechanisms of Pinholin Activation through Thermodynamic Integration and Mutational Analysis — ***Ted Kalbfleisch II***, *Vance Jaeger*

1:45 Paper 330f: Drug Resistance Predictions Based on Non-Equilibrium Alchemical Calculations — ***Matteo Aldeghi***, *Vytautas Gapsys, Bert de Groot*
1:58 Paper 330h: Variational Autoencoders As a Unifying Framework for Molecular Coarse Graining, Back-Mapping, and on-the-Fly Learning of Efficient Monte Carlo Moves — ***Jacob I. Monroe***, *Vincent K. Shen*
2:11 Paper 330i: Temperature-Transferable Coarse-Grained Modeling with Relative Entropy — ***Evan Pretti***, *M. Scott Shell*
2:24 Paper 330j: Replica Exchange and Backbone Sampling Methods Improve Protein-Protein Docking By Mimicking Induced-Fit Pathways — ***Ameya Harmalkar***, *Sai Pooja Mahajan, Jeffrey J. Gray*
2:37 Paper 330g: [Invited Talk] a Multiscale Simulation Approach for Formulation Design: Using Bottom-up Coarse Graining to Bridge All-Atom and Field Theory Simulations — ***Kevin Shen***, *My Nguyen, Nicholas Sherck, Brian Yoo, Stephan Kohler, Joshua Speros, Kris Delaney, M. Scott Shell, Glenn H. Fredrickson*

(331) Remediation of Emerging Contaminants and Legacy Compounds

Tuesday, Nov 9, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 308

Alexander Dowling, Chair
Sage Hiibel, Co-Chair
Robert Peters, Co-Chair

Sponsored by: Water

12:30 Paper 331a: Cyclic Adsorption and Persulfate Oxidation on Iron-Activated Activated Biochar for Removal of Microcystin-LR in Water and Wastewater — *Shengquan Zeng,* ***Eunsung Kan***
12:45 Paper 331b: Electrochemical Recycling N from Wastewater Towards Fossil-Free NH_3 Production Using Dispersed Ru Atom in Cu Metal Catalyst: An Ab-Initio Study. — ***Srishti Gupta***, *Daniel J. Rivera, Christopher L. Muhich*
1:00 Paper 331c: Identification of Environmental Microplastics Using Pyrolysis Gas Chromatograph Mass Spectrometry (Py-GC/MS) — ***Kerry Candlen***, *Gregory Reimonn, Wan-Ting Chen*
1:15 Paper 331d: Mesoporous Fe- or Cu-Doped MgO Nanoparticles for Photo-Fenton-like Degradation of Salicylic Acid — ***Manoj Silva***, *Jonas Baltrusaitis*
1:30 Paper 331e: Bisphenol a Degradation and Biofilm Formation By Engineering *Shewanella Oneidensis* — ***Jiacheng Zhou***, *Gregg P. Kotchey, David V. P. Sanchez,* ***Seok Hoon Hong***
1:45 Paper 746f: Sorption of Heavy Metal Ions By Composite Cryogels Based on Bentonite Clay with Ionic and Nonionic Polymer — ***Perizat Baimyrza***

(332) Soft systems, molecular simulation, sustainability

Tuesday, Nov 9, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 306

Carissa Eisler, Chair
Janani Sampath, Co-Chair

Sponsored by: Material Interfaces as Energy Solutions

12:30 Paper 332a: Polymer-guided interfacial assembly of nanoparticles into low-dimensional architectures — ***Gaurav Arya***, *Yilong Zhou, Tsung-Yeh Tang, Brian H. Lee*
1:05 Paper 332b: Soft and Stretchable Energy Harvesting Using Metal/Gel Interfaces — ***Veenasri Vallem***, *Erin Roosa, Tyler Ledinh, Michael D. Dickey*
1:24: Break
1:43 Paper 332d: Morphology and Charge Transport Predictions across Organic Photovoltaic Components Using Coarse-Grained Molecular Dynamics— *Mia Klopfenstein, Gwen White, Emily Elliston, Cody LaCoursiere, Cecily Martin, Nathanael Schwindt, James Rushing, Chris Jones, Jenny Fothergill, Michael Henry, Evan Miller, Matthew Jones,* ***Eric Jankowski***
2:02 Paper 332e: Exploring the Energy Landscape of Soft Glassy Systems— ***Amruthesh Thirumalaiswamy***, *Robert Riggleman, John C. Crocker*
2:21 Paper 332f: Optimized Generation of Initial Conformations for the Simulation of Amorphous Polymer Systems to Reduce Required Simulation Resources — *Nohemi D Trevino Garrido, Sahar Zenoozi, Clifford L. Henderson,* ***Peter J. Ludovice***
2:40 Paper 332g: Adaptive Grid-Based Method for Mapping Cavity Connectivity in Thermal Crystals and Amorphous Materials — ***Ryan Mullen***, *Nir Goldman, Tae Wook Heo, Kyle Sullivan, Brandon C. Wood*

(333) Special Session In Honor of Arup Chakraborty's 60th Birthday: Biology and Immunology

Tuesday, Nov 9, 12:30 PM
Marriott Copley Place, Salon C/D

Andrew Ferguson, Chair
Bernhardt L. Trout, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

12:30: Introductory Remarks
12:55 Paper 333b: Antigen Recognition at Immune-Cell Surfaces: Probing the Role of Mechanical Forces — ***Steven Abel***
1:20 Paper 333c: Bridging Statistical Inference and Stochastic Modeling to Shed Light on Gene Regulation — ***Elizabeth Read***
1:45 Paper 333d: On the Molecular Diversification and Maturation of Neurons in the Visual System — ***Karthik Shekhar***
2:10 Paper 333e: Multiscale Affinity Maturation Simulations to Elicit Broadly Neutralizing Antibodies Against HIV — ***Kayla Sprenger***, *Simone Conti, Victor Ovchinnikov, Arup K. Chakraborty, Martin Karplus*

(334) The Food-Energy-Water Nexus

Tuesday, Nov 9, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 311

M M Faruque Hasan, Chair
Vikas Khanna, Co-Chair
Yuan Yao, Co-Chair

Sponsored by: Sustainability Science and Engineering

12:30 Paper 334a: Life Cycle Assessment of Resource Recovery Technologies on Large-Scale Dairy Farms — ***Callan Glover***, *Pablo Cornejo, Sage Hiibel*
12:45 Paper 334b: Consumption-Based Accounting for Tracing Nutrient Footprints of Beef Supply Chains in the United States — ***Anais Ostroski***, *Oleg A Prokopyev, Vikas Khanna*
1:00 Paper 334c: Assessment of Global Water Stress Using the Generalized Global Sustainability Model (GSM) — *Neeraj Hanumante, Apoorva Nisal, Yogendra Shastri,* ***Urmila Diwekar***, *Heriberto Cabezas*
1:15 Paper 334d: Bacteria Containment in Filtration — ***Darryl Taylor***
1:30 Paper 334e: Use of the Aqueous Phase and Char from Hydrothermal Liquefaction of Biomass in Compost and Heavy Metal Adsorption Applications— ***Hengameh Bayat***, *Mostafa Dehghanizadeh, Catherine Brewer*
1:45 Paper 334f: Analysis of the Water-Energy-Food Nexus in Agriculture Dependent Rural Communities By Using Mathematical Programming — *Javier Garcia-Martinez,* ***Vicente Rico-Ramirez***, *Luis Fuentes-Cortés*
2:00 Paper 334g: Flue Gas (CO_2) Extraction and Bio-Sequestration (FGXB) for Increased Crop Yields and Water Utilization Efficiency (WUE) — ***Brian Kolodji***

(335) Theory, Modeling, and Simulation of Nuclear Chemical Processes

Tuesday, Nov 9, 12:30 PM
Marriott Copley Place, Salon A/B

Karl Hammond, Chair
Valmor de Almeida, Co-Chair

Sponsored by: Nuclear Engineering Division

12:30 Paper 335a: Molecular Dynamics Simulations of Hydrogen Retention in Single-Crystal and Polycrystalline Tungsten — ***Brandon Laufer***, *Karl Hammond*
12:51 Paper 335b: Mechanical Properties of Plasma-Exposed Tungsten — *Asanka Weerasinghe, Brian D. Wirth,* ***Dimitrios Maroudas***
1:12 Paper 335c: Effects of Elastic Softening and Surface Hole Formation on Surface Morphological Evolution in Plasma-Facing Tungsten — ***Chao-Shou Chen***, *Dwaipayan Dasgupta, Brian D. Wirth, Dimitrios Maroudas*
1:33 Paper 335d: Helium Aggregation Near Grain Boundaries in Plasma-Facing Tungsten — ***Karl Hammond***, *Dimitrios Maroudas, Brian D. Wirth*
1:54 Paper 335e: Soret Diffusion of Helium and Intrinsic Point Defects in Tungsten — ***Dimitrios Maroudas***, *Sophie Blondel, Brian D. Wirth, Enrique Martinez*
2:15 Paper 335f: A Revision of Classical Force Fields for Tri-*N*-Butil Phosphate Molecular Dynamics Simulations — ***Faranak Hatami***, *Valmor F. de Almeida*
2:36 Paper 335g: On the Onset of 'Fuzz' Formation in Plasma-Facing Materials: A Hierarchical Multiscale Modeling Approach — ***Dwaipayan Dasgupta***, *Asanka Weerasinghe, Sophie Blondel, Dimitrios Maroudas, Brian D. Wirth*

(336) Topical Plenary: Process Analytical Technology: Sensor Applications in Process Development (Invited Talks)

Tuesday, Nov 9, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 200

Ariel Furst, Chair
Jeffrey Halpern, Co-Chair

Sponsored by: Sensors

12:30: Introductory Remarks
12:35 Paper 336a: (Invited Plenary Talk) Silicon Nanowire Photoelectric Protein Sensors — ***Marcie Black***
1:10 Paper 336b: (Invited Plenary Talk) Glucose Sensors for Bioprocessing: Progress and Perspectives — ***Kenneth Reardon***
1:45 Paper 336c: (Invited Plenary Talk) Optical Sensing and Cell Culture— ***Stephen Grant***
2:20: Panel Discussion
2:40: Student Awardees Announcement
2:50: Business Meeting

(337) Transport In Advanced Fuel Cell Technologies

Tuesday, Nov 9, 12:30 PM
Sheraton Back Bay, Liberty B/C

Gang Wu, Chair

Sponsored by: Transport and Energy Processes

12:30: Break
12:55 Paper 337b: CFD-Based Modelling of an Open Flow Field Architecture Proton Exchange Membrane Fuel Cells — ***Mason (Mohsen) Benam***, *Filippo Gambini*
1:20: Break
1:45 Paper 337d: In-Line Analysis of Fuel Cell Materials – Detection and Impact of Defects in Membrane and Catalyst — ***Andrew Wagner***, *Thomas Lasko, Philip Cox*
2:10 Paper 337e: Highly Dispersion Nickel-Molybdate Bi-Metallic Nanoparticle on Cerium-Zirconium-Yttrium Support for SOFC Application — ***Mohamed Ali Elharati***, *Martinus Dewa, Steven R. Saunders, M. Grant Norton, Yohei Miura, Song Dong, Yosuke Fukuyama, Nilesh Dale, AbdulJabbar MohammedHussain, Su Ha*
2:35 Paper 337f: Metal-Supported Solid Oxide Fuel Cell System with Infiltrated Reforming Catalyst Layer Operating Under Direct Ethanol Feed Configuration— ***Martinus Dewa***, *Mohamed Ali Elharati, Yosuke Fukuyama, Yohei Miura, Song Dong, Nilesh*

Dale, AbdulJabbar MohammedHussain, M. Grant Norton, Su Ha

(338) Understanding the Rules of Life at the Micro- and Nano-Scale

Tuesday, Nov 9, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 109

Chang Liu, Co-Chair
Yuan Tang, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

12:30 Paper 338a: Target Search of Cas9 and Talen Is Dependent on Chromatin Architecture — ***Saurabh Shukla***, *Surbhi Jain, Charles M. Schroeder, Paul Selvin, Huimin Zhao*
12:48 Paper 338h: Microvasculature-on-a-Chip for Studying Endothelial Cell Pathophysiology — ***Yuan Tang***
1:06 Paper 338c: Nanoceria Morphology Dictates Metabolic Impairment in Primary Hepatocytes — ***Michael Moeller***, *Vaishaali Natarajan, Barry Cheung, Srivatsan Kidambi*
1:24 Paper 338d: Simulations of Electroenzymatic Glutamate Sensors in the Brain Reveal the Value of Finite Element Methods for Understanding Neurochemical Transmission — ***Mackenzie Clay***, *Harold Monbouquette*
1:42 Paper 338e: Multiplexed Three-Dimensional Protein Mapping — ***Yuxuan Tian***, *Chang Ho Sohn, Lauren DeLorenzo, Lee Kamentsky, Juhyuk Park, Kwanghun Chung*
2:00 Paper 338f: N-Terminal Derivatization-Assisted Identification of Individual Amino Acids Using a Biological Nanopore — *Xiaojun Wei, Qian Wang,* ***Chang Liu***
2:18 Paper 338g: Nanopore Tools for Probing Protein Dynamics and Sequence (Invited Speaker) — ***Meni Wanunu***

(339) Water Treatment, Desalination, and Reuse II

Tuesday, Nov 9, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 312

Oishi Sanyal, Co-Chair
Stephen Martin, Co-Chair
Lucy Mar Camacho, Co-Chair

Sponsored by: Membrane-Based Separations

12:30 Paper 339a: Water and Organic Co-Transport in Carbon Molecular Sieve Membranes — ***Young Hee Yoon***, *Ryan Lively*
12:52 Paper 339b: Improving Dye Removal Performance of Graphene Oxide Membranes By Etching and Polydopamine Intercalation — ***Xiaoyi Chen***, *Erda Deng, Xiaoci Lin, Lingxiang Zhu, Haiqing Lin*
1:14 Paper 339h: Produced Water and Waste Heat-aided Blowdown Water Treatment: Using Chemical and Energy Synergisms for Value Creation— ***Mohammad Hafez Ahmed***, *Payton Seats, Lian-Shin Lin*
1:36 Paper 339d: Investigation and Fabrication-Based Optimization of Polymeric Ultrafiltration Membrane Using Recycled PET and Green Solvent Components — ***David Lu***, *Parto Babaniamansour, Alex Williams, Isabel Escobar*
1:58 Paper 339e: Open-Access Database for Water Purification and Desalination Membranes — *Cody L. Ritt, Timothée Stassin, Douglas M. Davenport,* ***Ryan DuChanois***, *Ines Nulens, Zhe Yang, Naama Segev-Mark, Adi Ben-Zvi, Menachem Elimelech, Chuyang Y. Tang, Guy Z. Ramon, Ivo F. J. Vankelecom, Rhea Verbeke*
2:20 Paper 339f: Desalination and Separation of Oil-Saline Water Mixtures Utilizing Wettability and Photocatalysis Decoupled Membranes— ***Mohammadamin Ezazi***, *Mohammadamin Ezazi, Ki-yong Jee, Gibum Kwon*
2:42 Paper 339g: Evaluation of Integrated Electrocoagulation-Microfiltration and Direct Contact Membrane Distillation Processes for Produced Water Treatment— ***Ranil Wickramasinghe***, *M. G Jebur, Yu-Hsuan Chiao, Xianghong Qian*

(340) Meet the Industry Candidates Poster Session: Pharmaceutical Discovery, Development and Manufacturing Forum

Tuesday, Nov 9, 1:00 PM
John B. Hynes Veterans Memorial Convention Center, Exhibit Hall C/D

Moiz Diwan, Chair
Jasmine Rowe, Co-Chair
Nil Tandogan, Co-Chair

Sponsored by: Meet the Candidates Poster Sessions

Poster 340a: Quantifying Transient Metabolic Fluxes Using Stable Isotopes, Mass Spectrometry, and Computational Modeling — ***Cara L. Sake***, *Nanette Boyle, Keith B. Neeves*
Poster 340c: Utilizing Pyrolysis Secondary Gas-Phase Reactions to Produce Anisotropic Carbons from Non-Graphitizing Feedstocks — ***Joshua Malzahn***, *Ignacio Preciado, Eric Eddings*
Poster 340d: Solution Processing of Thin-Film Chalcogenide Solar Cell Materials — ***David Rokke***
Poster 340f: Application of Interfacial Rheological Techniques in Pharmaceutical Product Development — ***Sourav Barman***, *Joseph Zasadzinski*
Poster 340g: Optimizing Reaction Conditions and Zeolite Properties for Different Catalytic Applications — ***Deependra Parmar***
Poster 340h: Fluids-Based *in Vitro* Models for Disease and Development— ***Kiara Cui***, *Leeya Engel, Vincent Xia, Kevin Liu, Daniel Cirera Salinas, David Myung, Kyle Loh, Lay Teng Ang, Alexander R. Dunn, Gerald Fuller*
Poster 340i: Single Atom Catalysts for Oxidation - Understanding the Fundamentals of Synthesis and Reactivity — ***Shyam Deo***, *Linxi Wang, Nicholas Pantelis II, Kayla Eudy, Zayne Weber, Ahana Mukhopadhyay, Robert Rioux, Michael J. Janik*
Poster 340k: Understanding Solvent Effects in Catalysis and Adsorption in Metal Organic Frameworks — ***Roshan Ashokbhai Patel***, *Michael Tsapatsis, Joern Siepmann, Matthew Neurock*
Poster 340l: Studying the Effects of Mutations on the Structures and Binding of Therapeutic Proteins Towards Improving the Engineering of Protein Functions— ***Sumaiya Islam***, *Robert Pantazes*
Poster 340n: Development of Condition Monitoring Systems to Support Continuous Manufacturing of Pharmaceutical Oral Solid Dosages. — ***Rexonni Lagare***
Poster 340o: From Data to Decisions: Development of Surrogate Models for Process Optimization — ***Bianca Williams***
Poster 340p: Probing Interactions of Single-Walled Carbon Nanotubes at the Nano-Bio Interface — ***Mitchell Gravely***, *Daniel Roxbury*
Poster 340r: Design and Studies of CVD Graphene-Based Membranes on Modified Support for Water Treatment Applications — ***Mansour Saberi***, *Stephen Creager*
Poster 340s: Surface Engineering with Polymer Brush Thin Films Via Light-Mediated Polymerizations — ***Mingxiao Li***, *Christian Pester*
Poster 340u: Polycationic Hydrogel Nanocarriers for siRNA Delivery in Inflammatory Bowel Diseases — ***Aaliyah Shodeinde***
Poster 340w: Ionomers: Leading the Way to Electrochemical Devices — ***Seefat Farzin***
Poster 340z: Design and Development of Gold Nanoshell-Liposomes Formulations for Scalable, High-Throughput Ex-Vivo mRNA and DNA Delivery— ***Anisha Veeren***, *Joseph Zasadzinski*
Poster 340aa: Statistics, Data Science, and Molecular Modeling — ***Archit Datar***
Poster 340ab: Data-Driven Optimization of Dynamic Hybrid Models — ***William Bradley***, *Fani Boukouvala*
Poster 340ac: Peroxisome Engineering in the Oleaginous Yeast *Yarrowia Lipolytica and Expansions on Lessons Learned* — ***Michael Spagnuolo***
Poster 340ad: Multiscale Systems Engineering for the Development of Sustainable Technologies — ***Elvis Eugene***
Poster 340af: High-Throughput Passive Microrheological Screening of Gelation Conditions of Protein Hydrogels — ***Michael Meleties***, *Dustin Britton, Bonnie Lin, Priya Katyal, Jin Kim Montclare*
Poster 340ah: Bacteria As Active Colloids at Fluid Interfaces — ***Jiayi Deng***
Poster 340ai: Chemical Research and Development: *Process Modeling and Machine Learning* — ***Shiyan Wang***
Poster 340aj: Developing Tunable Solid Acid Catalysts — ***Andrew Wolek***, *Justin Notestein*
Poster 340am: Optimization Techniques for Pharmaceutical Manufacturing Processes through Design Space Analysis — ***Daniel Laky***
Poster 340an: Solvent Effects in Liquid-Phase Catalytic Reactions — ***Yanyu Mu***, *Robert Rioux*
Poster 340ao: Study of Water and Organic Co-Transport in Carbon Molecular Sieve Membranes — ***Young Hee Yoon***, *Ryan Lively*
Poster 340ap: *Pygran-Sim*: An Interoperability Tool for Running DEM Simulation— ***Andrew Abi-Mansour***
Poster 340aq: A Systematic Multiscale Computational Approach for Engineering Novel Adaptive Materials for Biological Applications— ***Sriramvignesh Mani***
Poster 340at: Development of Nanoemulsion-Loaded Hydrogels for Advanced Pharmaceutical Formulations — ***Liang-Hsun Chen***
Poster 340av: Engineering C_1 Reaction Chemistry through Catalyst Design and Process Intensification — ***Yifan Deng***, *Goetz Veser*
Poster 340aw: Fabrication of Inorganic Magnetic Nano-Composites for Biomedical Application — ***Sitong Liu***
Poster 340ax: Improving Charge Transfer in Metal Ions for Aqueous Redox Flow Batteries — ***Harsh Agarwal***
Poster 340az: On the Spatial Design of Co-Fed Amines for Selective Dehydration of Methyl Lactate to Acrylates — ***Yutong Pang***, *M. Alexander Ardagh, Manish Shetty, Anargyros Chatzidimitriou, Gaurav Kumar, Bess Vlaisavljevich, Paul Dauenhauer*
Poster 340bc: Design of Selective Palladium-Based Catalysts for Direct Synthesis of Hydrogen Peroxide — ***Tianze Xie***, *Robert Rioux*
Poster 340bd: Alpha Particle Nanotherapeutics Against Metastatic Triple Negative Breast Cancer — ***Aprameya Ganesh Prasad***
Poster 340be: Integrating Large Scale Systems Biology Data with Metabolic Modeling: A Chemical Engineering PhD Seeking Challenges in Computational Biology — ***Alexander Metcalf***, *Nanette Boyle*
Poster 340bf: Understanding & Correlating Atomic-Scale Compositions & Structures of Mesoporous N-Containing Carbon Electrocatalysts with Oxygen & Sulfur Reduction Properties — ***Shona Becwar***, *Bradley F. Chmelka*
Poster 340bg: Advancing Downstream Processes for the Purification of Therapeutic Viruses — ***Karina Kawka***, *Raja Ghosh, David Latulippe*
Poster 340bj: Investigation into Ion Transport Properties of Nanoparticle-Based Single-Ion Conducting Electrolytes Using Multiscale Simulations and Machine Learning — ***Sanket Kadulkar***, *Thomas Truskett, Venkat Ganesan*
Poster 340bk: Multiscale Modeling for Design of Responsive Soft Material Interfaces — ***Jonathan Sheavly***, *Reid Van Lehn*
Poster 340bm: Developing a Fully Closed Dbtl Cycle for Biosystems Design Via Automation and High-Throughput Screening — ***Pu Xue***
Poster 340bn: Unraveling the Role of Fe and Oxygen Defects on CoO_xnanoisland Structure and Water Splitting Activity Using Computational Approaches — ***Anthony Curto***, *Aleksandra Vojvodic*
Poster 340bs: Enzymatic Synthesis of Chemical Compounds.. — ***Karthik Sankaranarayanan***, *Chaitan Khosla*, Klavs Jensen**

Poster 340bu: Design of Antimicrobial Prodrugs Against Multidrug-Resistant Bacteria — ***Meghan O'Leary***, *Sabrina Chen, Lars Westblade, Christopher Alabi*
Poster 340bw: Three Biotherapeutic Case Studies: Manufacturing, Analytical Characterization, and Delivery — ***Srivatsan Ramesh***, *Ryan Smith, Christopher Gorman, Michael Daniele, Stefano Menegatti*
Poster 340bx: AI/ML for Predicting Oil Composition from Hydrothermal Liquefaction of Biomass — ***Seshasayee Mahadevan Subramanya***

(341) Academia-Industry Partnership: Preparing Students to be Leaders in Industry (Invited Talks)

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 302

Richard Braatz, Chair
Lucas J. Landherr, Co-Chair

Sponsored by: Bridging the Skills Gap in Chemical Engineering

3:30: Remarks from Roger Hart
3:50: Remarks from Patricia Hurter
4:10: Panel Discussion

(342) CoMSEF Poster Session

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, Exhibit Hall C/D

Jeetain Mittal, Chair
Kayla Sprenger, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

Poster 342f: Group Contribution and Machine Learning Approaches to Predict Abraham Solute Parameters, Solvation Free Energy, and Solvation Enthalpy— ***Yunsie Chung***, ***Pierre Walker***, *Florence Vermeire, Haoyang Wu, Michael Abraham, William Green*
Poster 342g: Inverse Design of Molecular Probes to Bind with Water Contaminants — ***Siva Dasetty***, *Yuqin Wang, Stuart J. Rowan, Sang Soo Lee, Seth B. Darling, Chris J. Benmore, Rebecca Willet, Eric Jonas, Junhong Chen, Andrew Ferguson*
Poster 342h: Excluded Volume Monte Carlo Simulations for Anisotropic Fluid Structure Predictions — ***Rizwanur Rahman***, *Michael P. Hoepfner*
Poster 342i: Machine Learning of Retrosynthetic Disconnections and Reaction Outcomes: Influence of Reaction Template Characteristics — ***Andrea Aude***, *Esther Heid, William Green*
Poster 342k: Mechanistic Insights into HIV Common Escape Pathways from Broadly Neutralizing Antibodies Via Molecular Dynamics Simulations— ***Jonathan Faris***, *Kayla Sprenger, Allen Lin, Alejandro Balazs*
Poster 342l: Workflow Development for First-Principles Molecular Simulations in CP2K — ***Ramanish Singh***, *Colin Bunner, Tyler Josephson, Ray Matsumoto, Peter Cummings, Joern Siepmann*
Poster 342m: DFT Study on Ag Loaded 2H-MoS_2 for Mechanism of Improved Photocatalytic Reduction of CO_2 — ***Xiaohong Yin***, *Feng Xin*
Poster 342n: Solidification Model for Silicon Crystal-Melt Interface in the Horizontal Ribbon Growth Process: A Molecular Dynamics Study — ***Victor Fabiyi***, *Eunsu Paek*
Poster 342p: First-Principles Study of the Role of Carbon Host in the Sodiation of Selenium — ***Sungwon Park***, *Eunsu Paek*
Poster 342q: Optimization of High-Throughput Photocatalyzed Bimetallic Nanoparticles Using Online Active Learning — ***Kirby Broderick***, *Eric Lopato, Zachary Ulissi, Stefan Bernhard*
Poster 342r: Structure-Property Relationships of Thiolate-Protected Metal Nanoclusters — ***Michael Cowan***, *Giannis Mpourmpakis*
Poster 342s: Gaining Mechanistic Insights into the Influence of O-Linked Glycosylation on Insulin Properties with Molecular Dynamics — ***Wei-Tse Hsu***, *Dominique Ramirez, Zhongping Tan, Tarek Sammakia, Michael Shirts*
Poster 342t: Si and C Models as the Basis for Regression-Driven Development of the Interface Force Field — ***Katarina Odak***, *Hendrik Heinz, Alan Weimer, Julie Nguyen*
Poster 342u: Altered Protein Dynamics Delineates the Oncogenic Potential of Various Kinase Mutations — ***Keshav Patil***, *Stanislav Y. Shvartsman, Ravi Radhakrishnan*
Poster 342v: Toward Data-Driven Approaches to Inverse Design: Fast and Accurate Evaluation of Gas Adsorption and Diffusivity in Nanoporous Materials— ***Musen Zhou***, *Jianzhong Wu*
Poster 342w: The Molecular Simulation Design Framework (MoSDeF): New Features to Improve User Experience and Support Reproducible Molecular Simulations — ***Nicholas C. Craven***, *Co Quach, Umesh Timalsina, Justin Gilmer, Ray Matsumoto, Parashara Shamaprasad, Arjun Bansal, Christopher Iacovella, Clare McCabe, Peter Cummings*
Poster 342x: Managing a High-Throughput Screening Workflow with Open-Source Software: A Study of Tribological Properties of Thin Films — ***Co D. Quach***, *Justin Gilmer, Christopher Iacovella, Peter Cummings, Clare McCabe*
Poster 342aa: Mathematical Modeling of the Observed Neutralization Threshold of Antibodies Against Sars-Cov-2 — ***Emily Rhodes***, *Tim Whitehead, Kayla Sprenger*
Poster 342ad: Computational Studies of the Phase Transitions and Self-Assembly of Thermoresponsive Peptide-Based Biomaterials — ***Phillip Taylor***, *April Kloxin, Arthi Jayaraman*
Poster 342ae: Accelerating on-the-Fly Active Learning of Catalyst Simulations Using Large Scale Pretrained Models — ***Joseph Musielewicz***, *Muhammed Shuaibi, Zachary Ulissi*
Poster 342af: Computational Analysis of Confined Deep Eutectic Solvents and Ionic Liquids for Separations of Carbon Dioxide from Methane — ***Jiaming Xu***, *Francisco Hung*
Poster 342ag: Molecular Dynamics Simulations of the Inhibition of HIV and Host Cell Machinery By Antiretroviral Drugs — ***Daisy Fuchs***, *Kayla Sprenger*
Poster 342aj: Predicting Rate Constants for Catalyzed Reactions with Machine Learning — ***Brenden Pelkie***, *Stephanie Valleau*
Poster 342ak: Predicting Uncertainty in Supervised Machine Learning Predictions of Chemical Kinetics — ***Evan Komp***, *Stephanie Valleau*
Poster 342al: Transforming Automated Quantum Chemistry Calculation Workflows with Machine Learning: Towards Faster and More Accurate Chemical Discovery — ***Chenru Duan***, *Heather Kulik*
Poster 342am: Improving Feature Selection Methods for Heterogeneous Catalysis — ***Chun-Yen Liu***, *Shengbin Ye, Meng Li, Thomas Senftle*
Poster 342an: Electronic Structure Modeling of Electric Field Driven Catalysis and Electrocatalytic Kinetics — ***Naveen Agrawal***, *Michael J. Janik*
Poster 342ap: Carbon-Chain Linked Solvated Electron Precursors: Role of an Adjustable Carbon-Chain on the Singlet-Triplet Energy Gap — ***Isuru Ariyarathna***
Poster 342aq: Estimation of the Binary Interaction Parameters of the Anrtl Model Using Molecular Simulations — ***Rajasi Shukre***, *Rajesh Khare, Chau-Chyun Chen*
Poster 342ar: DFT-Based Solvent Screening for Temperature Swing Solvent Extraction of High Salinity Brines — ***Xiaoyang Liu***, *Gabriel Barbosa, Steven Weinman, Jason Bara, C. Heath Turner*
Poster 342as: Theory and Simulation Studies of Structure and Thermodynamics in Polymer Blends and Polymer Nanocomposites with Directional Interactions — ***Arjita Kulshreshtha***, *Arthi Jayaraman*
Poster 342au: Ground and Excited Electronic States of Superalkalis: The Case of NLi_4, NNa_4, PLi_4, and PNa_4 — ***Isuru Ariyarathna***
Poster 342av: Molecular Dynamic Investigations of Thermodynamic and Transport Properties of Trinidad and Tobago Asphaltenic Heavy Oils — ***Festus Addo-Yobo***, *Adrian Lutchman*
Poster 342aw: Multimodal Integrated Modelling for COVID-19 Health Risk Management — ***Dimosthenis Sarigiannis***, *Ioannis Petridis, Achilleas Karakoltzidis, Spyros Karakitsios*
Poster 342ax: Epidemic Models with 'Time Since Infection': Efficient and Flexible Modeling Tools — ***Joseph Peterson***, *Ronojoy Adhikari*
Poster 342ay: Is Curvature Better? Examining the Structure of Nanoparticles Containing Curved Carbons — ***Kimberly Bowal***, *Jacob W Martin, Markus Kraft*
Poster 342az: Chain Topology Structure Simulation of Linear Low-Density Polyethylene Based on Graph Theory and Monte Carlo Algorithm — ***Jie Wang***
Poster 342bc: Molecular Dynamic Investigations of *E. coli* and *V. Cholerae* Fadl Homologs — ***Andrew Turgeson***, *Bradley Harris, David Giles*
Poster 342bd: Clean, High Quality Low Emission Transportation Fuels with Fischer-Tropsch Synthesis: A Mesoscale Study of Transport Processes in Confined Systems — ***Ioannis Economou***, *Konstantinos D. Papavasileiou, Loukas D. Peristeras, Andreas Bick*
Poster 342bf: Ensemble Dependence of Mechanical Relaxations and Their Underlying Correlation Functions — *Mason Hyde, Faramarz Joodaki,* ***Michael Greenfield***
Poster 342bg: Development of Accurate Coarse-Grained Models of Polar Organic Solvents — ***Soumil Joshi***, *Sanket Deshmukh*
Poster 342bh: Molecular Simulation Study of Deep Eutectic Solvent-Water Liquid-Liquid Interfaces — ***Usman Abbas***, *Qing Shao*
Poster 342bi: Relative Resolution: Implementation in Lammps of the Coulomb Potential — ***Aviel Chaimovich***
Poster 342bk: Deep Learning Molecular Force Field for Gaseous Adsorption in Metal-Organic Frameworks with Open-Metal Sites — *Chi-Ta Yang, Ishan Pandey,* ***Archit Datar***, *Chau-Chyun Chen, Joshua Howe, Li-Chiang Lin*

(343) General Poster Session in Sensors

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, Exhibit Hall C/D

Jeffrey Halpern, Chair

Sponsored by: Sensors

Poster 343a: Investigation of Electrochemical Redox Tags for Elastin-like Polymer Sensing — ***Stanley Feeney***, *Katherine Austin, Eva Rose M. Balog, Jeffrey Halpern*
Poster 343b: Mammalian Cell-Compatible "Light-up" RNA Aptamer Biosensors for Custom Small Molecule Targets — ***Everett Allchin***, *Ethan Lippmann*
Poster 343c: Microfabriction of GEM Sensors for Quantitative Glucose Mapping and Multiplexing with MRI — ***Mark Ferris***, *Samuel Oberdick, Gary Zabow*
Poster 343e: A Wearable Patch for Sweat Lactate Analysis — ***Tamoghna Saha***, *Jennifer Fang, Sneha Mukherjee, Michael D. Dickey, Orlin Velev*
Poster 343f: Evaluating the Fitness of Combinations of Adsorbents for Quantitative Gas Sensor Arrays — *Rachel Sousa,* ***Cory Simon***

(344) Interactive Session: Applied Mathematics and Numerical Analysis

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, Exhibit Hall C/D

Ali Mesbah, Chair
Satyajith Amaran, Co-Chair

Sponsored by: Applied Mathematics and Numerical Analysis

Poster 344a: A Logic-Based Modeling Study of the Immune Response Under High Glucose Conditions in Diabetic Kidney Disease — ***Krutika Patidar***, *Ashlee Ford Versypt*
Poster 344b: Field Wide Optimization Towards Improved Upstream Hydrocarbon Recovery — ***Shakeel Ramjanee***
Poster 344e: Ziegler and Nichols Meet Kermack and Mckendrick: Parsimony in Dynamic Models for Epidemiology — ***Michael Nikolaou***
Poster 344f: Feature Engineering and Machine Learning for Computer-Assisted Screening of Children with Speech Disorders — ***Farnaz Yousefi Zowj***, *Kerul Suthar, Marisha Speights Atkins, Q. Peter He*
Poster 344g: Novel Genetic Algorithm for Parameter Fitting Applied to Sigmoid Growth Models — ***Rex Gaumer***, *Kyle Camarda*
Poster 344h: A Kinetic Model of Plant Sphingolipid Metabolism Identifies Key Enzymes and Regulatory Interactions in the Pathway — ***Adil Alsiyabi***, *Rajib Saha*
Poster 344i: A Framework for Steady-State Process Operability Analysis Using Kriging-Based Surrogate Models — ***Victor Alves***, *Vitor Gazzaneo, Fernando V. Lima*
Poster 344j: Titles — ***Ahmet Demirtas***

(345) Interactive Session: Data and Information Systems

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, Exhibit Hall C/D

Kristen Severson, Chair

Sponsored by: Information Management and Intelligent Systems

Poster 345a: AI Speaker-Based Information Management and Multilingual Knowledge Service on Chemical Material Safety — ***Hunggi Lee***, *Sangwoo Yoo, MinKyoung Kim, Dongil Peter Shin*
Poster 345c: Data-Driven Dynamic Optimization Using Continuous-Time Surrogate Models — ***Burcu Beykal***, *Nikolaos A. Diangelakis, Efstratios N. Pistikopoulos*
Poster 345e: Prediction of Nitrous Oxide Concentration in Wastewater Treatment Plants: Application and Benchmarking of Deep-Learning Models — *Adem Rosenkvist Nielsen Aouichaoui, Sille Bendix Larsen, Mikkel Holmen Andersen,* ***Gürkan Sin***
Poster 345f: Feature Extraction for Process Monitoring with Nonstationary Measurements Based on Principal Component Analysis and Mutual Information— ***Cheng Ji***, *Zheng Lu, Xuebing Zhu, Fangyuan Ma, Jingde Wang, Wei Sun*
Poster 345g: A Modified Bayesian Network to Handle Cyclic Causal Network in Root Cause Diagnosis of Rare Events — ***Pallavi Kumari***, *Qingsheng Wang, Joseph Kwon*
Poster 345i: A Comparative Analysis on Interpretability of Explainable AI (XAI) for Neural Network Based Fault Detection Methods — ***Suyeon Sohn***, *Jay H. Lee*
Poster 345k: A Functional Safety System That Prescribes Optimal Time-Varying Proactive Actions — ***Masoud Soroush***, *Leila Samandari Masooleh, Ulku Oktem, Warren Seider, Jeffrey E. Arbogast*
Poster 345l: Decision Template-Based Fusion of Multiple Classifiers for Fault Detection in Chemical Process — ***Bairi Sai Vasista***, ***Abhijit Bhakte***,***Rajagopalan Srinivasan***
Poster 345m: Fitting of Failure Models with Bathtub-Shaped Failure Rate to Data Using Optimization Algorithms — ***Teemu Ikonen***, *Francesco Corona, Iiro Harjunkoski*
Poster 345o: Data-Driven and Knowledge Hybrid Real-Time Decision Making for Exposed Chemical Hazard Based on Knowledge Graph Inference Expanded By Deep Learning — ***Sangwoo Yoo***, *Hunggi Lee, En Sup Yoon, Dongil Peter Shin*
Poster 345p: Machine Learning Assisted Prediction Modelling for Pressure Vessel Design and Stress Analysis. — ***Abdulfatai Faro***, *Kazeem Salam, Dare Jeremiah,* ***Aonullahi Adebayo***, ***Oluwapemi Adekanmi***
Poster 345q: Classification of Cardiomyocyte Content Differentiated from Human Induced Pluripotent Stem Cells — ***Samira Mohammadi***, *Ferdous Finklea, Mohammadjafar Hashemi, Bianca Williams, Elizabeth Lipke, Selen Cremaschi*
Poster 345r: An Efficient Reinforcement Algorithm Approach to Stochastic Optimal Control with Application to Biodiesel Production. — ***Shiam Kannan***, *Urmila Diwekar*
Poster 345s: An Integrated Machine Learning and Optimization Approach for Octane Optimization — ***Metin Turkay***, *Ahmet Can Serfidan*
Poster 345u: A Machine Learning Approach for the Design of a Soft Sensor in an Oil Refinery's Distillation Column — ***Jimena Ferreira***, *Martín Pedemonte, Ana I. Torres*
Poster 345v: Reinforcement Learning of Optimization Strategy and Horizon Length Selection in Online Vehicle Routing — ***Teemu Ikonen***, *Keijo Heljanko, Iiro Harjunkoski*
Poster 345w: Machine Biology for Infectious Diseases — ***Cesar de la Fuente-Nunez***

(346) Interactive Session: Systems and Process Control

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, Exhibit Hall C/D

Cara Touretzky, Chair
Fernando V. Lima, Co-Chair

Sponsored by: Systems and Process Control

Poster 346d: Community Detection for Distributed Control — *Leila Samandari Masooleh, Jeffrey E. Arbogast, Ulku Oktem, Warren Seider,* ***Masoud Soroush***
Poster 346a: Asymmetric Model Predictive Control Strategies for Blood Glucose Control — ***Travis Diamond***, *Faye Cameron, B Wayne Bequette*
Poster 346b: Modeling and Analysis of Endogenous Closed-Loop Control of the Cardiovascular System — ***Michelle Gee***, *Eden Hornung, Alison Moss, Lakshmi Kuttippurathu, James S. Schwaber, Babatunde A. Ogunnaike, Rajanikanth Vadigepalli*
Poster 346c: Machine Learning Applications in Prediction of Propagation Rate Coefficients of Acrylate-Based Polymers for Electronics Applications — ***Tung Nguyen***, *Mona Bavarian*
Poster 346e: Advanced Process Control of Methanol Production from Natural Gas — ***Md Emdadul Haque***, *Peter Nazier, Srinivas Palanki*
Poster 346g: Simulation of Morphological Population Balance for Crystallization Processes Using Cellular Automata — ***Jiali Ai***, *Chi Zhai, Jindong Dai, Wei Sun*
Poster 346h: *Setting the "PACE" with Advanced Process Control* — ***Leticia de Souza Zarpellon***
Poster 346j: A Hybrid Mechanistic-Machine Learning Approach to Identify Dynamical Models for Sustainability Assessment of Manufacturing Processes: A Soybean Diesel Process Case Study — ***William Farlessyost***, *Shweta Singh*
Poster 346m: Learning Partial Differential Equations from Multiscale or Experimental Data: A Showcase on Bacterial Chemotaxis — ***Georgios Psarellis***, *Seungjoon Lee, Sujit Datta, Ioannis G. Kevrekidis*
Poster 346n: Reinforcement Learning with Neural Feedback Policies — *Ilya Orson Sandoval Cárdenas,* ***Panagiotis Petsagkourakis***, *Antonio del Rio Chanona*
Poster 346p: Chemometric Techniques for the Combined Calibration/Parameter Estimation of Pharmaceutical Drug Substance Manufacture — ***Daniel Casas-Orozco***, *Daniel Laky, Jaron Mackey, Ahmed Mufti, Gintaras V. Reklaitis, Zoltan Nagy*
Poster 346r: Field Wide Optimization Towards Improved Hydrocarbon Recovery— ***Shakeel Ramjanee***
Poster 346s: Data-Driven Distributionally Robust Optimization for Process Control — ***Panagiotis Petsagkourakis***, *Antonio del Rio Chanona, Zhengang Zhong*
Poster 346u: Gsvd Carleman State Estimation of Nonlinear Discrete-Time Systems with Gross Errors — ***Gbolahan Dada***, *Antonios Armaou*

(347) Interactive Session: Systems and Process Design

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, Exhibit Hall C/D

Bhavik Bakshi, Chair
Matthew Realff, Co-Chair

Sponsored by: Systems and Process Design

Poster 347b: Modeling, Engineering, and Integration of a Smart Moisture Absorbing Foam (SMAF) into a Man-Portable Atmospheric Water Extraction Device — ***Travis Emery***, *Peter Warren, Sean Torrez, John Kidd, Jacob Miske, Tiffany Yu, John Grimble, Todd Emrick, Ian Norris, Paul Smith, David Gamliel*
Poster 347d: Multi-Level Modelling of Low-Carbon Heating Systems: Integrating Household-Level Cost-Benefit Analysis with National-Level Value Chain Optimisation — ***Jennifer Penman***, *Sheila Samsatli*
Poster 347e: Energy Integration for Waste Heat in Industrial Plants through a Metaheuristic-Deterministic Approach — *Francisco J. López-Flores Sr., Luis Germán Hernández-Pérez,* ***Luis Fernando Lira-Barragán III***, *Eusiel Rubio-Castro, Jose Ponce-Ortega*
Poster 347f: A Recycle/Reuse Network for the Optimal Water Management in Hydraulic Fracturing Operations — *Tania I. Serrano-Arevalo Jr.,* ***Luis Fernando Lira-Barragán III***, *Jose Ponce-Ortega, Mahmoud El-Halwagi*
Poster 347h: Simulation-Based Comparison between Three Different Clean-in-Place Configurations Regarding Their Cleaning Efficiency and Water Use— ***Hossam Metwally***, *Muhammad Sami, Kathleen Brown*
Poster 347i: Laser-Irradiated Holey Graphene-Supported Single-Atom Catalyst Towards Hydrogen Evolution and Oxygen Reduction — ***Kishwar Khan***, *Zhengtang Luo, Khalil Amine*

(348) Interactive Session: Systems and Process Operations

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, Exhibit Hall C/D

Ruth Misener, Chair
Dimitrios Georgis, Co-Chair
M M Faruque Hasan, Co-Chair

Sponsored by: Systems and Process Operations

Poster 348a: A Procedure for Identifying a Nearly Pareto-Optimal Operation Policy for Pressure Swing Adsorption Processes — ***Taehun Kim***, *Joseph K. Scott*
Poster 348b: Field Wide Approach to Optimization for Improved Hydrocarbon Recovery — ***Shakeel Ramjanee***
Poster 348d: The Lambert Function Should be in the Engineering Mathematical Toolbox — ***Iordanis Kesisoglou***, ***Garima Singh***, *Michael Nikolaou*
Poster 348e: A Homotopy Continuation-Based Branch and Bound Algorithm for Strongly Nonconvex Mixed Integer Nonlinear Programming Problems in Process Synthesis — ***Yingjie Ma***, *Nan Zhang, Jie Li*
Poster 348f: An Integrated Prediction and Process Optimization Software Platform for Highly Efficient Neural Network Development in Chemical Engineering and Related Fields — ***Dela Quarme Gbadago***, *Jiyoung Moon, Sungwon Hwang*
Poster 348h: Quantum Integer Programming: An Open-Access Practical Guide and Toolkit for Novel Computational Paradigms for Optimization — ***David E. Bernal***, *Sridhar Tayur, Davide Venturelli*

(349) Poster Session: Advances in Zeolite Science and Technology

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, Exhibit Hall C/D

Robert Saxton, Chair

Sponsored by: Advances in Zeolite Science and Technology

Poster 349a: Harnessing Heteroatom Effects in Zeolite Synthesis: A Kinetic Trap for Organic-Free FAU — ***Adam J. Mallette***, *Sungil Hong, Emily Freeman, Sarah A. Saslow, Sebastian Mergelsberg, Radha Kishan Motkuri, James Neeway, Giannis Mpourmpakis, Jeffrey Rimer*
Poster 349b: Unique Roles of Heteroatoms in the Zeolite Synthesis— ***Deependra Parmar***, *Adam Mallette, Lars Grabow, Jeffrey Rimer*
Poster 349c: Thermodynamic Analysis of the Reversible Interconversion of Platinum Cations to Nanoparticles in SSZ-13 Zeolites — ***Anupama Jayaraman***, *Keka Mandal, Christopher Paolucci*
Poster 349e: Predicting Relative Stabilities of Divalent Cations in Metal-Exchanged Zeolites — ***Asanka Wijerathne***, *Christopher Paolucci*
Poster 349f: Chemoselective Characterization of Brønsted Acid Site Accessibility Using Probe Amine Uptake in Infrared Spectroscopy— ***Choongsze Lee***, *Heng Dai, M. Alexander Ardagh, Jeffrey Rimer, Michael Tsapatsis, Paul Dauenhauer*
Poster 349i: Catalytic Site Design for Lewis Acid Zeolites for the Epoxide Ring Opening with Alcohols — ***Alexander Spanos***, *Nitish Deshpande, Aamena Parulkar, Nicholas Brunelli*
Poster 349j: Synthetic Approaches to Independently Vary Crystallite and Atomic-Scale Acid Site Distributions and Their Catalytic Consequences for Propene Oligomerization — ***Elizabeth Bickel***, *Hannah McGinness, Claire Nimlos, Natalie Zamiechowski, Rajamani Gounder*
Poster 349k: Reaction Calorimetry for Adsorption Thermodynamics in Zeolite— ***Ajibola Lawal***, *Omar Abdelrahman*
Poster 349l: Solvatation of the Hofmann Elimination of Alkylamines through Cooperative Adsorption — ***Han Chen***, *Omar Abdelrahman*
Poster 349m: Tuning the Interaction of Molecules with Lewis Acid Zeolite By Hot Carriers — ***Tien Le***, *Bin Wang*
Poster 349n: On the Spatial Design of Co-Fed Amines for Selective Dehydration of Methyl Lactate to Acrylates over NaY Zeolite Catalyst — ***Yutong Pang***, *M. Alexander Ardagh, Manish Shetty, Anargyros Chatzidimitriou, Gaurav Kumar, Bess Vlaisavljevich, Paul Dauenhauer*
Poster 349o: A DFT and Microkinetic Modeling Study of Confinement Driven Diels-Alder Reactions in Acidic Zeolites — ***Christopher Rzepa***, *Srinivas Rangarajan*
Poster 349q: Cooperative Adsorption: Solvating the Hofmann Elimination of Alkylamines — ***Han Chen***, *Omar Abdelrahman*
Poster 349r: Tuning Electronic Properties of Active Sites for Alkene Epoxidations with H_2O_2 — ***E. Zeynep Ayla***, *David Potts, Daniel Bregante, David Flaherty*
Poster 349s: Understanding the Influence of Chain Length, Branching, and Void Environment on the Stability of Surface-Bound Alkyl Intermediates in Zeolites Using DFT — ***Lauren Kilburn***, *Mykela DeLuca, David Hibbitts*
Poster 349x: The Effect of Non-Crystalline Al Species on Catalytic Performance of H-ZSM5 Zeolite — ***Vy Nguyen***, *Tram Pham, Steven Crossley, Bin Wang*
Poster 349y: How Do the Building Blocks of Zeolites Grow? — ***Sungil Hong***, *Adam Mallette, Radha Kishan Motkuri, James Neeway, Jeffrey Rimer, Giannis Mpourmpakis*
Poster 349z: Spatiotemporal Coke Coupling Enhances Para-Xylene Selectivity in Highly Stable MCM-22 Catalysts — ***Deependra Parmar***, *Seunghyeok Cha, Taha Salavati-fard, Ankur Agarwal, Jeremy Palmer, Lars Grabow, Jeffrey Rimer*
Poster 349aa: Studies on Hydrocarbon Diffusion and Accessibility in FCC Catalysts — *Francisco Murilo T. Luna,* ***Celio Cavalcante Jr.***, *Eduardo Falabella Sousa-Aguiar, José Marcos M. Ferreira*
Poster 349ad: Roles of Interaction between Components in Czza/HZSM-5 Catalyst for Dimethyl Ether Synthesis Via CO_2 Hydrogenation — ***Xiao Fan***, *Baitang Jin, Shoujie Ren, Shiguang Li, Miao Yu, Xinhua Liang*
Poster 349ae: A Novel Method of 3D Printing High-Loaded Oxide/H-ZSM-5 Catalyst Monoliths for Propane to Propylene Conversion — *Shane Lawson,* ***Kyle Newport***, ***Daniel Hanify***, ***Fateme Rezaei***, ***Ali Rownaghi***
Poster 349af: Mesoporous Zeolites Supported Catalysts for Selective Ring Opening of 1-Methylnaphthalene with Remarkably Enhanced BTEX Yield — ***Ke Zhang***, *Michael Forte, Essam Al-Sayed*
Poster 349ag: A Kinetic Modelling Strategy for Interrogating NOx Selective Catalytic Reduction on Cu-Exchanged Zeolites — ***Anshuman Goswami***, *Siddarth Krishna, Yujia Wang, Casey B. Jones, Rajamani Gounder, William Schneider*
Poster 349ah: Structure-Property Relationship of Metal Encapsulated in MFI Zeolites for CO Hydrogenation — ***Jane Agwara***, ***Marc Porosoff***
Poster 349aj: A Multimodal XAFS and DFT Study of the Sulfur Adsorption Sites in Cu and Ce Ion-Exchanged Y Zeolite — ***Henry Sokol***, *Kevin Lee, Anatoly I. Frenkel, Stavros Caratzoulas, Julia A. Valla*
Poster 349ak: Methane Oxidation on Pd/SSZ-13 Active Sites: A Computational Study — *Kevin Giewont, Eleni Kyriakidou,* ***Eric Walker***

(350) Poster Session: Chemical Engineering Education

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, Exhibit Hall C/D

Christy West, Chair
J. Patrick Abulencia, Co-Chair

Sponsored by: Education

Poster 350a: Integrating Student-Created STEM Comics into Chemical Engineering Education — ***Lucas Landherr***
Poster 350b: Student-Generated Wikis As an Assessment Tool — ***J. Patrick Abulencia***
Poster 350c: Gamification of Quantitative Problems to Increase Student Engagement — ***John Wagner***

(351) Poster Session: Fuels and Petrochemicals Division

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, Exhibit Hall C/D

Paul Mathias, Chair

Sponsored by: Fuels and Petrochemicals Division

Poster 351a: The Case of the Missing Asphaltenes from the Naphthenic Froth Treatment Process — ***Weiyi Kong***, *Jeffery S. Job, Michael P. Hoepfner*
Poster 351c: Microwave-Assisted Dehydrogenation of Ethane over Stable Csru/CeO_2 Catalyst for Production of Light Olefins — ***Xiaoyan Wang***, *Yuxin Wang, Jianli Hu*
Poster 351d: Thermochemical gas splitting using iron aluminate-based materials — ***Justin Tran***, *Carter Wilson, Kent J. Warren, Alan Weimer*
Poster 351g: Comparison of the Technologies Utilized for Refining of the Utilized Lubricating Oil — ***Saish Pawar***, *Dr. Utkarsh Maheshwari*

(352) Poster Session: Fundamentals and Applications of Adsorption and Ion Exchange

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, Exhibit Hall C/D

Masoud Jahandar Lashaki, Chair
Sasidhar Gumma, Co-Chair

Sponsored by: Adsorption and Ion Exchange

Poster 352a: Developing Amine-Grafted Silica Materials for CO_2 Capture from Enclosed Environments — *Sara Ahsan, Ali Ayub,* ***Masoud Jahandar Lashaki***
Poster 352b: Made-to-Order Amine-Grafted Silica Materials for Concurrent Removal of Carbon Dioxide and Water Vapor from Landfill Gas — *Ali Ayub, Sara Ahsan,* ***Masoud Jahandar Lashaki***
Poster 352c: An Investigation into Electrospun Scaffolds Containing Ion-Exchange Resins for Direct Capture of CO2 from Ambient Air — ***Kevin Chen***, *Jennifer Weiser, Amanda Simson*
Poster 352d: Design and Development of Smart Moisture Absorbing Foams for Atmospheric Water Extraction — ***Caitlin Bien***, ***Cameron McConnell***, *Dorin Preda, John Kidd, Russell Lambert, Zachary Whitermore, Tiffany Yu, Jeffrey Yee, Bryan E. Sharkey, Todd Emrick, Ian Norris, Paul Smith, David Gamliel*
Poster 352f: Henry Constants of Krypton on 4A, 5A and 13X and Saturation Loadings on 5A and 13x Zeolites — *Dana Abouelnasr,* ***Kevin Loughlin***

BREAK

(353) Poster Session: General Topics on Separations

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, Exhibit Hall C/D

Joshua Thompson, Chair

Sponsored by: General Topics and Other Methods

Poster 353a: Recycling Americium from Spent Nuclear Fuel through Molten Salt Electrodeposition — ***Bethany Kersten***, *Krista Hawthorne, Mark Williamson, Rohan Akolkar, Christine Duval*
Poster 353b: The Best of Both Worlds: Combining Advanced Polymer Chromatography with Advanced Multi-Detection for Complete High-Resolution Polymer Characterization — ***Ragy Ragheb***
Poster 353c: Field Deployable Kit for Removal of Aromatic Hydrocarbon and Heavy Metal Contaminants from Firefighter Turnout Gear — ***Russell Lambert***, *Dorin V. Preda, Min Song, David Gamliel*
Poster 353e: Bioactive Bacterial Cellulose Membranes Loaded with Frutalin Lectin (*Artocarpus incisa* L.) — *Thamyres Da Silva, Fabia K. Andrade, Celio Cavalcante Jr., Andre L. C. Silva,* ***Rodrigo Silveira Vieira***

(354) Poster Session: Membrane Separations

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, Exhibit Hall C/D

Mahdi Malmali, Chair

Sponsored by: Membrane-Based Separations

Poster 354c: "Click"-Crosslinkable CO_2-Philic Crosslinking of Poly(ethylene glycol) (PEG) Based Membranes for Natural Gas Separations — ***Dana Wong***, *John Yang, Sipei Li, Yang Liu, Seth Sharber*
Poster 354d: Molecular Dynamics Simulations Probe Greenhouse Gas Sorption Capabilities of Metal-Organic Framework-Based Membrane for Efficient Gas Separation Processes — ***Jordan Chapman***, *Nagasree Garapati, Vassiliki-Alexandra Glezakou, Yuhua Duan, Jianli Hu, Cerasela Zoica Dinu*
Poster 354g: Beta-Barrel Membrane Protein-Based Biomimetic Nano-Porous Membrane for Protective Fabrics — ***Hyeonji Oh***, *Yu-Ming Tu, Manish Kumar, Benny D. Freeman*
Poster 354h: Covalent Polymer/Inorganic Hybrids Membranes for Gas — ***Sipei Li***, *John Yang, Dana Wong, Yang Liu*
Poster 354k: Membranes for Point of Care Sensors — ***Leslie Thomas***, *Erica Forzani, Mary Lind*
Poster 354l: Catalytically Active Asymmetric Membranes for Reduction of 4-Nitrophenol — ***Yingxin He***, ***Ali Rownaghi***
Poster 354p: Process Design of Onboard Membrane Carbon Capture and Liquefaction Process to Satisfy the

Eedi Phase 5 — ***Juyoung Oh***, *Rahul Anantharaman, Umer Zahid, PyungSoo Lee, Youngsub Lim*
Poster 534c: Modeling Vibratory Nanofiltration System for Coffee Extract Preconcentration — ***Michael Vincent Laurio***, *C. Stewart Slater, Mariano J. Savelski, Kirti Yenkie, Robert Hesketh, Ramon Christian Eusebio*
Poster 534h: Process Simulation and Technoeconomic Analysis of Black Liquor Concentration with Graphene Oxide Membranes — ***Zhongzhen Wang***, *Chen MA, Scott A. Sinquefield, Sankar Nair*

(355) Poster Session: Separations Division

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, Exhibit Hall C/D

Ranil Wickramasinghe, Chair
Deepak Sharma, Co-Chair

Sponsored by: Separations Division

Poster 355a: Synthesis of a Heptazine-Based Polyhedral Oligomeric Silsesquioxane Framework for Adsorption Applications — ***Dana Abdullatif***, *Ahmadreza Khosropour, Alireza Abbaspourrad*
Poster 355b: Synthesis of Polyamide Reverse Osmosis Membranes for Separating Small Neutral Charged Molecules — ***Shahriar Habib***, *Steven Weinman*
Poster 355c: Membranes Containing Amines and Amino-Functionalized Multi-Walled Carbon Nanotubes for CO_2/H_2 Separation — ***Yutong Yang***, *Ruizhi Pang, Yang Han, Winston Ho*
Poster 355d: High Performance Blend Membranes Based on Poly(arylene ether sulfone) and Poly(styrene-isobutylene-styrene) for Direct Methanol Fuel Cell Applications — ***Gilberto Ramos Rivera***, *David Suleiman*
Poster 355e: Fabrication of Highly Permeable Matrimid Substrates for a CO_2-Selective Composite Membrane — ***Ruizhi Pang***, *Kai Chen, Yang Han, Yutong Yang, Winston Ho*
Poster 355f: CO_2 Utilization Via Solid Oxide Fuel Cells Enabled By a CO_2 -Selective Membrane — ***Ruizhi Pang***, *Yang Han, Winston Ho*
Poster 355g: Animated Interactive Data Visualization Tool for Pressure Swing Adsorption Simulations — ***Jack Tabb***, *Taehun Kim, Joseph K. Scott*
Poster 355h: Effect of Nanopatterning on Concentration Polarization during Nanofiltration in Direct Flow Studies — ***Lauren Ward***, *Barbara Fickling, Steven Weinman*
Poster 355i: Scale-up of Facilitated Transport Membranes for Hydrogen Purification from Coal-Derived Syngas — ***Yang Han***, *Yutong Yang, Ruizhi Pang, W.S. Winston Ho*
Poster 355j: Techno-Economic Analysis of Facilitated Transport Membranes for H_2 Purification from Coal-Derived Syngas — ***Yang Han***, *W.S. Winston Ho*
Poster 355l: Chiral Purification of *L*-Menthol By a New Technique Combining Melt Crystallization and Vaporization — ***Lie-Ding Shiau***
Poster 355m: Intensified Water Purification Via Carbon Dioxide-Mediated Diffusiophoresis — ***Esai Lopez***, *Patryck Michalik, Elizabeth Stewart, Andrew R Teixeira*
Poster 355n: Mixtures of Amino Acid Salts and Ethylene Glycol for CO_2Capture — ***Aidan Klemm***, *Burcu Gurkan*
Poster 355o: Separation of Ternary Refrigerant Mixtures Using Extractive Distillation with Ionic Liquid Entrainers — ***Ethan Finberg***, *Kalin Baca, Abby Harders, Andrew Yancey, Mark Shiflett*
Poster 355p: Remarkable Effect of Low Loading of Metal-Organic Polyhedra on Gas Separation Properties of Cross-Linked Polyethers — ***Taliehsadat Alebrahim***, *Liang Huang, Heshali Welgama, Vincent Pastore, Timothy R. Cook, Haiqing Lin*
Poster 355q: Advances in Single Use Centrifuge , Unifuge, Technology for Viral Vectors, VLP, Vaccines and Stem Cell Processing — ***David Richardson***
Poster 355s: Planar Micro-Contactors for Electric-Field-Enhanced Separation of Valuable Chemicals from Complex Reaction Mixtures — *Anna Kasparova, Alexandr Romanov, Lucie Vobecka, Zdenek Slouka,* ***Michal Pribyl***

(356) Poster Session: Thermodynamics and Transport Properties (Area 1A)

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, Exhibit Hall C/D

Andrew Paluch, Chair
Diwakar Shukla, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

Poster 356a: Experimental Investigation of Enhancing Oil Recovery for Umm Niqa Heavy Oil — *Ahmad Al-Shammari, Osamah Alomair,* ***Adel Elsharkawy***
Poster 356b: Evaluation of Thermal Conductivities for Liquid Mixtures Using Asog-Thermconduct Model — ***Katsumi Tochigi***, *Hiroyuki Matsuda, Kiyofumi Kurihara, Toshitaka Funazukuri*
Poster 356c: Evaluation of Solid-Liquid Equilibria for Drug + Water + Cyclodexstrins System Using Activity Coefficient Models — ***Katsumi Tochigi***, *Hiroyuki Matsuda, Kiyofumi Kurihara*
Poster 356h: Thermodynamics of Fe-Doped Magnesium Manganate for Thermochemical Energy Storage — ***Jayni Hashimoto***, *Alicia Bayon, Christopher L. Muhich*
Poster 356k: Ionic Solvation in Dual-Zwitterion Electrolytes: A Molecular Simulation Study — ***Manh Tien Nguyen***, *Qing Shao*
Poster 356o: The Phase Diagram of a Biomimetic Polymer during Force Spectroscopy — ***Aviel Chaimovich***
Poster 165ad: Characterization of Glycocalyx Components in Human Endothelial Cells — ***Theodora Stanley***, ***John Mwangi***, ***Selina Banerjee***, *Ronodeep Mitra, Eno Ebong*

(357) Poster Session: Transport and Energy Processes Division

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, Exhibit Hall C/D

Gus Georgeton, Chair

Sponsored by: Transport and Energy Processes

Poster 357b: Enhanced Durability of $Li_{1.2}Mn_{0.54}Co_{0.13}Ni_{0.13}O_2$ Cathode Material By Slightly Fluorinated Al_2O_3 ALD Coating — ***Han Yu***, *Xinhua Liang*
Poster 357c: Mass Transport Optimization in Direct Formic Acid Fuel Cell Catalyst Layer Via Pore-Former Templating — ***Steven Lam***, *Cynthia Ann Rice*
Poster 357d: Thermal Conductivity of Imidazolium Ionic Liquids Saturated with Compressed Gases — ***Karim Al-Barghouti***
Poster 357e: Fabrication and Testing of Asymmetric Supercapacitors Fabricated with (Mn,Ti)-Oxides and Chtl Derived Hydrochar/Graphene — ***Khang Huynh***, *Bharath Maddipudi, Vinod Amar, Anuradha Shende, Rajesh Shende*

(358) Advanced batteries II

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 306

Charles B. Musgrave, Chair
Griselda Bonilla, Co-Chair

Sponsored by: Material Interfaces as Energy Solutions

3:30: Break
3:51: Break
4:12 Paper 358e: *Electrosprayed Scalable 3D Graphene-CNT Electrodes for Li-Ion and Fuel Cell Applications* — ***Caspar Yi***, *Enoch Nagelli, Sophia Tarpey, Danielle A. Lynch, Duncan Day, Jordan M. Davis, F. John Burpo, Preston Haney, Harry L. Moore*
4:33 Paper 358f: Modeling the Brønsted Acidity of Lanthanum Exchanged Faujasite — ***Richard Shiery***, *Stuart McElhany, David Cantu*
4:54 Paper 358g: Charge Transport Mechanism in Sodium Selenide (Na_2Se) for Sodium-Selenium Batteries: A First Principles Study — ***Sungwon Park***, *Eunsu Paek*
5:15: Break
5:36 Paper 47c: Nitrogen-Rich Free-Standing Carbon Cathode for Improved Lithium-Sulfur Battery Performance — ***Jeongwoo Yang***, *Jae Hyun Park, Won Yeong Choi, Dohyeun Kim, Hyeonseo Gim, Jae Lee*

(359) Advances in Algae Cultivation, Conversion and Products

Friday, Nov 19, 12:30 PM
Virtual, Sustainable Engineering Forum (23)

Sridhar Viamajala, Chair
Lynn Wendt, Co-Chair

Sponsored by: Sustainable Biorefineries

12:30: Break
12:51 Paper 359b: Application of Membrane CO_2 Absorber in NH_4oh Looping Process for Enhanced Algae Growth — ***Feng Zhu***, *Xiaoshuai Yuan, Aaron Smith, Mark Crocker, Heather Nikolic, Kunlei Liu*
1:12 Paper 359c: Co-Product Recovery in Wet Anaerobic Storage to Reduce the Cost of Algae Biomass for Fuels and Chemicals Production — ***Bradley Wahlen***, *Hongqiang Hu, Birendra Adhikari, Lynn Wendt*
1:33 Paper 359d: Simulations of Mixing and Radiative Interactions in Large-Scale Raceway Ponds for Algae Cultivation. — ***John Parra-Alvarez***, *Hariswaran Sitaraman, Mohammad J. Rahimi, Jonathan Stickel, Lieve Laurens, Ruby Carrillo, Mark Deimund, Sarah Feicht, Joseph Weissman*
1:54 Paper 359e: A Fed-Batch Mixotrophic Cultivation Strategy for Enhanced Biomass Growth and Metabolite Formation — ***Gonzalo Figueroa-Torres***, *Jon Pittman, Constantinos Theodoropoulos*
2:15 Paper 359f: Integrated Conversion of Algal Biomass to Fusel Alcohols and Optimization of Alcohol Mixture Composition for Maximum Fuel Economy/Efficiency in Light Duty Vehicles — ***Eric Monroe***, *Lily Behnke, Ryan Davis, Fang Liu*
2:36 Paper 359g: Efficient Resource Recovery to Enhance Biomass Conversion— ***Yupo Lin***, *Jian Liu, Charles J. Freeman, Michael R. Thorson*

(360) Advances in New Modalities (Large Molecule, Oligos, Peptides, ADCs, Gene therapy, etc.) Product and Process Development (includes invited talks)

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 101

Boung Wook Lee, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

3:30 Paper 360a: Analysis of Transformed Bioprocess Data and Application of Hybrid Modeling Approaches to Enhance Upstream Process Development— ***Kristina Mathis***, ***Boung Wook Lee***, *Dave Stevenson*
3:54 Paper 360b: Challenges in the Pharmaceutical Development of Lipid Nanoparticle Therapeutics — ***Nelia Viza***, *Angela Wagner, Yong Liu, Agnes Zhao, Amy Doty, Katelyn Smith, Xiujuan Jia, Jameson Bothe, Yongchao Su, Mingyue Li, Eric Kemp, Adam Socia, Erin Guidry, Marian Gindy*
4:18: Break
4:42 Paper 360e: Dynamic Optimization of an Ultrafiltration System for the Concentration of Monoclonal Antibody Solutions Under Uncertainty— ***Francesco Rossi***, *Jessica Zuponcic, Eduardo Ximenes, Steven Geng, Yinying Tao, Vincent Corvari, Michael Ladisch, Gintaras V. Reklaitis*
5:06 Paper 360f: Confocal Imaging of Protein Gel Layer Formation during Tangential Flow Filtration to Inform Process Conditions Reducing Protein Losses and

Increasing Protein Concentration — *Jessica Zuponcic, Francesco Rossi, Eduardo Ximenes, Norvin Bruns, Steven Geng, Yinying Tao, Vincent Corvari, Gintaras V. Reklaitis,* ***Michael Ladisch***

(361) AIChE Management Award Recipient Presentation Session -How to Attract, Develop and Sustain Engineering Expertise Needed by Industry

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 301

Joseph Cramer, Chair
George Newcomb, Co-Chair
Harold Conner Jr., Co-Chair

Sponsored by: Management Division

3:30 Paper 361a: Award Presentation to Senyo Opong — ***Joseph Cramer,George Newcomb****, Harold Conner Jr.*
3:40 Paper 361b: Developing and Sustaining Critical Engineering Knowledge and Expertise in a Rapidly Changing World — ***Senyo Opong***
4:20 Paper 361c: Lessons from the Renewal of a Corporate Technology Organization — ***William Raiford***
4:50 Paper 361d: Chemical Engineers in the Pharmaceutical Industry — ***Jean Tom***
5:20 Paper 361e: Management an easy mountain to climb? … really?— ***Markus Scheller***
5:50 Paper 361f: Q & A of all speakers — ***George Newcomb****,* ***Joseph Cramer****, Harold Conner Jr.*

(362) Andrew Chase Award (Invited Talks)

Tuesday, Nov 9, 3:30 PM
Marriott Copley Place, Provincetown

Xuejun Pan, Chair

Sponsored by: Forest and Plant Bioproducts Division

3:30 Paper 362a: Biomass Derived Sustainable Materials and High-Performance Devices — ***Hongli Zhu***
4:00 Paper 362b: Progress in Thermochemical Production of Cellulosic Sugars— ***Robert Brown***
4:30 Paper 362c: Single-Use Plastic Wastes: Challenges and Sustainable Alternatives — ***Amar K. Mohanty***

(363) Anisotropic Particles: Synthesis, Characterization, Modeling, Assembly, and Applications

Tuesday, Nov 9, 3:30 PM
Sheraton Back Bay, Back Bay Ballroom A

Isaac Torres Diaz, Chair
Bhuvnesh Bharti, Co-Chair

Sponsored by: Interfacial Phenomena

3:30 Paper 363a: Solution-Based Fabrication and Application of Tunable Particles for Surface-Enhanced Raman Scattering — ***Tania Oliveira****, Akram Abbasi, Irene Andreu Blanco, Arijit Bose*
3:45 Paper 363b: Chloride Directs the Growth of Cu Nanowires — ***Junseok Kim****, Jianming Cui, Kristen Fichthorn*
4:00 Paper 363d: Dynamic Magnetochromatic Response of Concentrated Suspensions of Janus Particles — ***Jinghui Gao****, Samuel Wilson-Whitford, James Gilchrist*
4:15 Paper 363e: Self-Assembly of Plasmonic Chiral Superstructures on Substrate By Circularly Polarized Light — ***Ji-Young Kim****, Connor McGlothin, Minjeong Cha, Emine Sumeyra Turali-Emre, Nicholas Kotov*
4:30 Paper 363f: Topological DLVO Interactions of Spiky Particles with a Planar Substrate — ***Isaac Torres Diaz****, KaiLian Davis*
4:45 Paper 363g: Competing Structural Motifs in Confined Assemblies of Hard Tetrahedral Particles — ***Rachael Skye****, Julia Dshemuchadse*
5:00 Paper 363h: Anomalous Dynamics of Rigid Convex Particle Shapes — ***Thi Vo****, Vyas Ramasubramani, Joshua Anderson, Sharon Glotzer*
5:15 Paper 363i: Fabrication and Investigation of Shape-Controlled Tri-Layer Graphene Particles at Fluid-Fluid Interfaces — *David M. Goggin, Amy Chacon,****Joseph Samaniuk***
5:30 Paper 363j: Progress Toward Colloidal Robotics — *Albert Tianxiang Liu, Jing Fan Yang,* ***Allan Brooks****, Volodymyr Koman, Ge Zhang, Daichi Kozawa, Sungyun Yang, Michael S. Strano*

(364) Applications of Data Science in Molecular Sciences II

Tuesday, Nov 9, 3:30 PM
Marriott Copley Place, Salon H/I

Andrew Ferguson, Chair
Johannes Hachmann, Co-Chair
Andrew White, Co-Chair

Sponsored by: Applications of Data Science to Molecules and Materials

3:30 Paper 364a: Analytical Methods to Improve Diagnostic Protocols Using Infrared Spectroscopic Imaging — ***Shachi Mittal****, Jonathan Kim, Rohit Bhargava*
3:42 Paper 364b: Message Passing Neural Networks for Prediction of IR Spectra — ***Charles J. McGill****, Michael Forsuelo, Yanfei Guan, William Green*
3:54 Paper 364c: Transfer Learning for Prediction of Absorption and Emission Spectra from Multi-Fidelity Data — ***Kevin P. Greenman****, William Green, Rafael Gomez-Bombarelli*
4:06 Paper 364d: Multi-Task Property Prediction: Importance of the "Chemist-in-the-Loop" in Model Building — ***Adem Rosenkvist Nielsen Aouichaoui****, Seyed Soheil Mansouri, Jens Abildskov, Gürkan Sin*
4:18 Paper 364e: Specific Ion Effects in Aqueous Electrolyte Solutions from First Principles-Derived Machine-Learning Potentials — ***Shuwen Yue****, Athanassios Panagiotopoulos*
4:30: Break
4:42 Paper 364g: Combining Molecular Dynamics Simulations and Active Learning to Study the Hydrophobicity of Chemically Heterogeneous Surfaces— ***Atharva Kelkar****, Bradley C. Dallin, Reid Van Lehn*
4:54: Break
5:06 Paper 342e: Machine Learning the COSMO Model for Predicting Thermodynamics of Electrolyte Mixtures — ***Eric Fonseca****, Ashwin Ravichandran, Richard G. Hennig, John W. Lawson*
5:18 Paper 364j: Generating 3D Conformer Ensembles of Molecular Graphs with End-to-End Differentiable Networks — ***Lagnajit Pattanaik****, Octavian Ganea, Connor Coley, Regina Barzilay, Tommi S. Jaakkola, Klavs F. Jensen, William Green*
5:30 Paper 364k: Graph Invariants As Rapid Features for Classification and Regression of Bulk Hydrogen Intercalation Energies in Reducible Metal Oxides— ***Evan Miu****, James R. McKone, Giannis Mpourmpakis*
5:42 Paper 364l: Something Old, Something New: Generative Adversarial Approaches to Conditional Sampling in Complex System Simulations — *Juan Bello-Rivas,* ***Ellis Crabtree****, Andrew Ferguson, Ioannis G. Kevrekidis*

(365) Biofuels Production: Design, Simulation, and Economic Analysis

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 311

Ramalingam Subramaniam, Chair
Ana I. Torres, Co-Chair

Sponsored by: Sustainable Biorefineries

3:30 Paper 365a: Technoeconomic Analysis of a Microalgae-Based Biorefinery Network for the Production of Advanced Biofuels — ***Gonzalo Figueroa-Torres****, Constantinos Theodoropoulos*
3:45 Paper 365b: Simulation and Life Cycle Assessment of Biodiesel Production from Micro Algae — ***Ramalingam Subramaniam****,* ***Ian Ivey****, Jade Young, Srinivasan Ambatipati*
4:00 Paper 365c: Techno-Economic and Sensitivity Analysis of Aromatic and Alkene Production from Lignin Via Fast Pyrolysis and Catalytic Upgrading Coupled with Ethanol Production. — ***Alvina Aui****, Alireza Saraeian, Yu Gao, Mark Mba Wright, Marcus Foston, Brent H. Shanks*
4:15 Paper 365d: Machine-Learning Reduced Order Model for Cost and Emission Assessment of a Pyrolysis — ***Olumide Olafasakin****, Yahan Chang, Alberto Passalacqua, Shankar Subramaniam, Robert Brown, Mark Mba Wright*
4:30 Paper 365e: Evaluation of the Economic Viability and Sustainability of Autothermal Pyrolysis Sugars through Computation and Machine Learning— ***Arna Ganguly****, Robert Brown, Mark Mba Wright*
4:45 Paper 365f: A Comparative Modeling Analysis of Electromicrobial Production Process Strategies — ***Anthony Abel****, Jeremy Adams, Douglas S. Clark*
5:00 Paper 365g: Middle Distillates from Ethanol-Technoeconomic and Life CYCLE Assessment — ***Juan Manuel Restrepo-Florez****, Paolo Cuello Penaloza, Emmanuel Canales, George Huber, Christos Maravelias*
5:15 Paper 365h: Investigation of Suitable Technologies & Solvents for Bio-Ethanol Dehydration with the Help of Aspen. — ***Saksham Pathrol****, Muskaan Lahariya, Vikas Kumar Sangal*

(367) Characterization of Biomaterials and Biological Systems

Tuesday, Nov 9, 3:30 PM
Sheraton Back Bay, Constitution B

Danielle Mai, Chair
Michelle Calabrese, Co-Chair

Sponsored by: Fluid Mechanics

3:30 Paper 367j: Characterizing the Heterogeneity of Stem Cell Populations Useful for Transplantation — *Tunglin Tsai, Shubha Tiwari, Clarissa C. Ro, Andrew Yale, Lisa A. Flanagan,* ***Tayloria Adams***
3:45 Paper 367a: Diffusion of Knotted DNA Molecules in Nanochannels in the Extended De Gennes Regime — ***Zixue Ma****, Kevin Dorfman*
4:00 Paper 367c: High-Throughput Microrheology of Synthetic and Biomolecular Polyelectrolytes Using Differential Dynamic Microscopy — ***Yimin Luo****, Mengyang Gu, Yue He, Chelsea Edwards, Megan T. Valentine, Matthew Helgeson*
4:15 Paper 367d: Investigating the Impact of Bond Exchange Kinetics on the Injectability of Dynamic Covalent Hydrogels — ***Anne Crowell****, Thomas FitzSimons, Eric V. Anslyn, Adrianne Rosales*
4:30 Paper 367e: Design of Thermo-Responsive Biopolymer Gels for Formulation and Delivery of Epidermal Growth Factors — ***Gianna Villani****, Olivia Eskens, Samiul Amin*
4:45 Paper 367f: Determining How Human Mesenchymal Stem Cells Change Their Degradation Strategy in Response to Microenvironmental Stiffness — *Maryam Daviran, Jenna A. Catalano,* ***Kelly Schultz***
5:00 Paper 367i: Systematic *in silico* Investigation of Blood Rheology and Thixotropy — ***Elahe Javadi****,* ***Safa Jamali***

(368) Design and Analysis of Carbon Capture and Negative Emissions Technologies - Models

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 309

Omar Guerra, Chair
Dora Lopez De Alonzo, Co-Chair

Sponsored by: Climate Change

3:30 Paper 368a: Cryogenic Separation of CO_2, SO_2, and NO_x from Flue Gas— ***Mohammed Sadaf Monjur****, Mark Holtzapple, M M Faruque Hasan*

3:45 Paper 368b: Optimization and Analysis of Carbon Capture in Ethanol Biorefineries — ***Caleb Geissler***, *Christos Maravelias*
4:00 Paper 368d: Steady State and Dynamic Modeling of a Flexible Carbon Capture-Equipped Power Plant Integrated with Lime-Based Direct Air Capture.— ***Moataz Sheha***, *Edward Graham, Dharik Mallapragada, Emre Gençer, Phillip Cross, James Custer, Adam Goff, Ian Cormier, Howard Herzog*
4:15 Paper 368f: Why Global Cooperation Will be Needed to Achieve Carbon Dioxide Removal at the Paris Agreement's Scale — ***Solene Chiquier***, *Mathilde Fajardy, Niall Mac Dowell*
4:30 Paper 368g: Determining the Role of Negative Emission Technologies (NETs) in the Electricity System in the UK — ***Augustin Prado***, *Mathilde Fajardy, Niall Mac Dowell*
4:45: Break

(369) Division Plenary: Food, Pharmaceutical, and Bioengineering Division (Invited Talks)

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 109

Sponsored by: Food, Pharmaceutical & Bioengineering Division

3:30 Paper 369a: Computational protein design as a tool for insight, discovery, and surveillance — ***Costas D. Maranas***
4:20 Paper 369b: Using RNAs as a built-in sensors of cell biology — ***Lydia M. Contreras***
5:10 Paper 369c: Engineering Microbial Nitrogen Delivery to Cereals— ***Christopher A. Voigt***
5:35 Paper 369d: Bioengineering beyond cells to enable a fair and sustainable 21st bio-century — ***Michael Jewett***
6:00 Paper 369e: Unlocking Intracellular Therapeutic Targets Using Bioinspired Materials — ***Millicent O. Sullivan***

(370) Education Division Awards Plenary (Invited Talks)

Tuesday, Nov 9, 3:30 PM
Sheraton Back Bay, Republic Ballroom B

Benjamin Davis, Chair
Matthew Liberatore, Co-Chair

Sponsored by: Undergraduate Education

3:30: Welcoming Remarks
3:35 Paper 370b: In Honor of the 2020 Education Division Award Winner for Innovation in Chemical Engineering Education — ***Daniel Burkey***
4:05 Paper 370a: In Honor of the 2019 Education Division Award Winner for Innovation in Chemical Engineering Education. — ***Peter J. Ludovice***
4:35 Paper 370c: In Honor of the 2020 Education Division Award for Service to Chemical Engineering Education — ***Stephanie Farrell***
4:50: Panel Discussion

(371) Electrochemical Fundamentals: Faculty Candidate Session II

Tuesday, Nov 9, 3:30 PM
Sheraton Back Bay, Commonwealth

Matthew Gebbie, Chair
Wenzhen Li, Co-Chair

Sponsored by: Electrochemical Fundamentals

3:30 Paper 371a: Bridging Length Scales in Electrolyte Transport Theory Via the Onsager Framework — ***Kara Fong***, *Kristin Persson, Bryan McCloskey, Kranthi K. Mandadapu*
3:50 Paper 371b: Mechanistic Understanding of Electrochemical Processes in Alkaline Environments — ***Roberto Schimmenti***, *Saurabh Bhandari, Ellen A. Murray, Manos Mavrikakis*
4:10 Paper 371c: Using Surface Thermochemistry and Band Alignment to Stabilize Interfaces in Solid-State Batteries — ***Robert Warburton***, *Jeffrey Greeley*
4:30 Paper 371d: Control of Nanoparticle Interfaces for Electrocatalytic Applications — ***Dohyung Kim***
4:50 Paper 371e: Breaking Aliphatic Carbon-Carbon Bonds Via Electrochemically Mediated Hydrogen Atom Transfer Reactions and Its Application to Polystyrene Deconstruction — ***Bing Yan***, *Changxia Shi, Eugene Y.-X Chen, Gregg T. Beckham, Yuriy Roman*
5:10 Paper 371f: A First Principles Analysis of the Potential-Dependent Reaction Mechanism of Ethanol Electrooxidation on Pt(100) — ***Siddharth Deshpande***, *Jeffrey Greeley*

(372) Enabling Technologies Relevant to Drug Substance and Drug Product III

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 102

David Am Ende, Chair
Dana Barrasso, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

3:30 Paper 249a: End-to-End Reconfigurable Process Development for the Cancer Drug Lomustine — ***Jaron Mackey***, *Ahmed Mufti, Devna Grover, Alex Harris, Joshua Prahlow, Gabriella Pruneda, Mesfin Abdi, Xin Feng, Erin Wood, Vivian Wang, David H. Thompson, Zoltan Nagy*
3:54 Paper 249f: Continuous Recycling of an Immobilized Biocatalyst in a Solids Forming Reaction By Magnetic Separation — *Matthew McDonald, Grant Marshall,* ***Colton Lagerman***, *Martha Grover, Ronald Rousseau, Andreas Bommarius*
4:18 Paper 372b: Spray Drying Proteins: Advances in Process Understanding Using the Model Protein Human Serum Albumin — ***Daniela Fiedler***, *Ulrich Kaindlbauer, Elisabeth Fink, Isabella Aigner, Eva Roblegg, Johannes G. Khinast*
4:42 Paper 372a: Novel Vaginal Pessary Platform Via 3D-Printing: Concomitant Mechanical Support and Drug Delivery — *Simone Eder, Laura Wiltschko,* ***Ioannis Koutsamanis***, *Florian Arbeiter, Eva Roblegg, Martin Spörk*
5:06 Paper 372f: Detecting and Evaluating Irregular Objects in OCT Images with Unsupervised Machine Learning — ***Elisabeth Fink***, *Anna Peter, Vanessa Herndler, Sandra Stranzinger, Matthias Wolfgang, Phillip Clarke, Johannes G. Khinast*

(373) Engineered Particles and Nanostructured Particulate Systems Characterization

Tuesday, Nov 9, 3:30 PM
Sheraton Back Bay, Fairfax A/B

Maria Tommassone, Chair

Sponsored by: Particle Production and Characterization

3:30 Paper 373a: Spray Drying of Drug Loaded Nanoparticles with Matrix Forming Excipients — ***Nicholas J. Caggiano***, *Robert K. Prud'homme, Rodney Priestley*
3:45 Paper 373b: Methods for Encapsulating Mobile Microparticles — ***Samuel Wilson-Whitford***, *Jinghui Gao, Maria Chiara Roffin, Thitiporn Kaewpetch, James Gilchrist*
4:00 Paper 373c: Magnetic Nanomaterial Endocytosis: Uptake and Cytotoxicity— *Chen Zhou,* ***Abhinav Sannidhi***, *Paul W. Todd, Thomas R. Hanley*
4:15 Paper 373d: Engineering Nanostraws for MCM-41 Microparticles Towards Enhancing the Adsorption of Guest Molecules: Application in CO_2 Capture.— ***Azeem Farinmade***, *Oluwole Ajumobi, Lei Yu, Julia A. Valla, Daniel F. Shantz, Vijay T. John*
4:30 Paper 373e: Characterizing Graphene Oxide Suspensions with Rheological Testing and Modeling, Neutron Scattering, and Electrochemical Performance — ***Matthew Armstrong***, *Enoch Nagelli, Ryan P. Murphy, Benjamin Thompson, Katie Weigandt, Jeffrey Chin, Simuck Yuk, F. John Burpo, Gabriela Huggins, Taylor Vessel, Andrew Mackey, Kevin Brooks, Lucas McCleery*

(374) Fuel and Energy Decarbonization

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 305

Eric Tan, Chair
Nixon Sunny, Co-Chair
William Barrett, Co-Chair

Sponsored by: Sustainable Energy

3:30 Paper 374a: Life-Cycle Analysis of Low-Carbon Hydrogen Supply Pathways for the Provision of Heat in Buildings — ***Nixon Sunny***, *Piera Patrizio, Niall Mac Dowell*
3:55 Paper 374b: Decarbonizing Industrial Heat: The Potential of Low Carbon Technologies in Chemicals Manufacturing — ***Carrie Schoeneberger***, *Jennifer B. Dunn, Eric Masanet*
4:20 Paper 374c: Green Hydrogen from PEM Electrolysis: Uncovering Its Worldwide True Cost and Production Boundaries When Accounting for Intermittency — ***Diego Freire***, *Andres Gonzalez Garay Sr., Thorsteinn Halfdanarson, Caroline Ganzer, Piera Patrizio, Niall Mac Dowell*
4:45 Paper 374d: Comprehensive Process and Environmental Impact Analysis of Integrated DBD Plasma Based Fuel Synthesis — ***Jonas Baltrusaitis***
5:10 Paper 374e: Low-Pressure Microwave Assisted Ammonia Synthesis – Evaluation of Novel Separation Technologies, Plant-Wide Process Design, and Technoeconomic Analysis — ***Opeyemi Ogunniyan***, *Chirag Mevawala, Yuxin Wang, Debangsu Bhattacharyya, Jianli Hu*
5:35 Paper 59c: National Priorities in the Net-Zero Transition of Electricity Systems: Policy and Technology Dimensions — ***Yoga Wienda Pratama***, *Niall Mac Dowell*

(375) Future of Manufacturing and Emerging Technologies

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 201

You Peng, Chair
Matthew Ellis, Co-Chair

Sponsored by: Next-Gen Manufacturing

3:30 Paper 375a: Multiscale Modeling of Spray Coating of Perovskite QDs: Understanding the Role of Molecular Interactions in Particle Aggregation.— ***Niranjan Sitapure***, *Joseph Kwon*
3:50 Paper 375b: Findings and Conclusions from a Mobile Worker and Augmented Reality Enabled Continuous Manufacturing Skid Project. — ***Iiro Esko***, *Katelyn Kelsey, Andrew Nachenberg, Leon Grossman*
4:10: Break
4:30 Paper 375d: Practical Issues in Cybersecurity: From Encryption to Images— ***Dominc Messina***, *Kathryn Tyrrell, Minhazur Rahman, Kip Nieman, Keshav Kasturi Rangan, Henrique Oyama, Samantha Cherney, Arlan Bonislawski, Helen Durand*
4:50 Paper 375e: Keynote Talk: Machine Learning and AI Applications in the Chemical Industry — ***You Peng***, *Leo Chiang*
5:25 Paper 375f: Keynote Talk: Deploying AI for Automated Monitoring of Physical Infrastructure — ***Prateek Joshi***

(376) Graduate Student Award Session: Inorganic Materials

Wednesday, Nov 17, 8:00 AM
Virtual, Materials Engineering and Sciences Division (08)

Xueyi Zhang, Chair
Kumar Varoon Agrawal, Co-Chair

Sponsored by: Inorganic Materials

8:00 Paper 376a: Characterization of Open-Metal Site Density and Speciation in Mixed-Valence Trimetallic Nodes of Metal-Organic Framework MIL-100— ***Jacklyn Hall***, *Praveen Bollini*
8:20 Paper 376b: The Interrelationship between Lanthanide and Actinide Dopants and the Local Environments on the Luminescent Properties of Complex Metal Oxide — ***Yuming Wang***, *James Dorman*
8:40 Paper 376c: Novel Study on Mixed Ultra-Thin Films of Titanium and Zirconium Oxides on Titanium Implant Abutment Surfaces Using Atomic Layer Deposition — ***Mina Shahmohammadi***, *Paul Sung, Bin Yang, Christos G. Takoudis*
9:00 Paper 376d: Multi-Objective Optimization for Selective Atomic Layer Deposition: A Case Study with Zirconia Deposition on Silicon Copper Composite. — ***Soumya Saha***, *Rajib Mukherjee, Christos G. Takoudis, Urmila Diwekar*
9:20 Paper 376e: Machine Learning Guided Synthesis of Multinary Chevrel Phases for Tunable Energy Materials — ***Nick Singstock***, *Charles B. Musgrave*
9:40 Paper 376f: AI-Accelerated Synthesis of Targeted Nanoparticle Heterostructures Using Agent-Based Sequential Learning — ***Carolin Wahl***, *Muratahan Aykol, Jordan Swisher, Joseph Montoya, Santosh Suram, Chad A. Mirkin*
10:00 Paper 376g: Highly Porous $Ti_3C_2T_x$ Mxene-Based Fibers Via Interfacial Complexation — ***Farivash Gholamirad***, *Nader Taheri-Qazvini*

(377) Highly Selective Separations with Membranes II

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 111

Dibakar Bhattacharyya, Co-Chair
Christine Duval, Co-Chair

Sponsored by: Membrane-Based Separations

3:30 Paper 377a: Facilitated Transport Membrane with Ionic Liquid and Poly(ionic liquid) Carriers for CO2 Separation from Air — ***Yun-Yang Lee***, *Burcu Gurkan*
3:45 Paper 377b: Facilely Cross-Linking Polybenzimidazole with Polycarboxylic Acids to Enhance H_2/CO_2 Selectivity — ***Leiqing Hu***, *Haiqing Lin*
4:00 Paper 377c: Membrane NH_3 Separation from N_2 and H_2 at High Temperature Close to the Haber-Bosch Process — ***Huazheng Li***, *Surya Padinjarekutt, Shoujie Ren, Miao Yu*
4:15 Paper 377d: Simultaneous Separation of CO_2 and H_2S from Natural Gas By Modified Poly(ether-*block*-amide) Membranes — ***John Yang***, *Milind Vaidya, Sebastien Duval, Garba Yahaya, Feras Hamad, Essam Al-Sayed, Ahmed Bahamdan*
4:30 Paper 377e: High-Silica CHA-Type Zeolite Membranes for Dehydration of Acetic Acid — ***Shaowei Yang***
4:45 Paper 377f: Permeability, Solubility, and Diffusivity of HFC-32 and HFC-125 in Polymeric Membranes — ***Abby Harders***, *Erin Sturd, Mark Shiflett, Thao Nguyen*
5:00 Paper 377g: Amine-Containing Membranes with Functionalized Multi-Walled Carbon Nanotubes for CO_2/H_2 Separation — ***Yutong Yang***, *Yang Han, Ruizhi Pang, Winston Ho*

(378) Hydrocarbon Conversion: Light Alkane Dehydrogenation and Aromatization

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 205

Joshua Howe, Chair
Sukaran S. Arora, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

3:30: Break

3:48 Paper 378b: Metal Exchanged Chabazite Zeolite for Non-Oxidative Dehydrogenation of Ethane — ***Jian Pan***, *Raul Lobo*
4:06 Paper 378c: Zinc Promoted Pt/ZSM-5 Catalysts for Ethane Dehydroaromatization — *Genwei Chen, Siavash Fadaeerayeni, Rudane Griffiths, Hossein Toghiani,* ***Yizhi Xiang***
4:24 Paper 378d: Tin-Exchanged Siliceous Supports for Propane Dehydrogenation — ***Natalie Lefton***, *Alexis T. Bell*
4:42 Paper 378e: Computational Characterization and Screening of Metal Phosphidesfor Ethane Dehydrogenation — ***Jeonghyun Ko***, *William Schneider*
5:00 Paper 378f: Identifying Alkane Dehydrogenation Metal-Oxide Catalysts through Lewis Acid-Base Strengths — ***Mona Abdelgaid***, *Giannis Mpourmpakis*
5:18 Paper 378g: First Principles Analysis of Selectivity and Durability of Pt-Based Bimetallic Alloys for Light Alkane Dehydrogenation — ***Yinan Xu***, *Ranga Rohit Seemakurthi, Zhenwei Wu, Jeffrey T. Miller, Jeffrey Greeley*
5:36 Paper 378h: Ethylene Production Using Oxidative Dehydrogenation with an M1 Catalyst: Effects of Membrane Separation & NOVEL Distillation Technologies — *Anne Gaffney, Ashton Aleman, Kaitlyn M. Cook, Austin B. Daniel, Robert D. Dodson Jr., Gillian O. Donnelly,* ***Kenneth Roberts***, *Yousif Alcheikhhamdona, Mina Hoorfar, Bo Chen, Sudip Majumdar, Hannah Murnen*

(379) Hydrogel Biomaterials: Emerging Applications

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 105

Murat Guvendiren, Chair
Marjan Rafat, Co-Chair
Adam Ekenseair, Co-Chair
Amir Sheikhi, Co-Chair

Sponsored by: Biomaterials

3:30 Paper 379a: Polymer Nanoparticle Hydrogels for Improved Cell Transplantation — ***Abigail Grosskopf***, *Gillie A. Roth, Emily Gale, Joseph Mann, Hector Lopez Hernandez, Eric A. Appel*
3:48 Paper 379b: Fiber-Based Protein Hydrogel As a Vehicle for the Topical Application of Therapeutic Exosomes — ***Michael Meleties***, *Priya Katyal, Juan Cortes Troncoso, Joseph Kuhn, Bonnie Lin, Bibi Subhan, Iraines De la Cruz, Piul Rabbani, Jin Kim Montclare*
4:06 Paper 379c: Mechanical Characterization, Release and Degradation of Hyaluronic Acid-Methyl Cellulose Thermogels for Viable Mitochondria Replacement Therapy — *Brian Duggan,* ***M. Arif Khan***, *Maliha A. Marium, Daniel Darby, Krishnaroop Chaudhuri, Felicia Michael, Jonathan Pham, Samir P. Patel, Jason E. DeRouchey, Alexander G. Rabchevsky, Thomas D. Dziubla*
4:24 Paper 379e: Polymeric Foams Capable of Arresting Bleeding from Non-Compressible Injuries — ***Hema Choudhary***, *Michael B. Rudy, Matthew B. Dowling, Srinivasa R. Raghavan*
4:42 Paper 379f: Dietary Fiber-Inspired Hydrogels for Removal of Uremic Toxins— ***Matthew Garnett***, ***Symone Alexander***
5:00 Paper 379g: Electroadhesion of Polyelectrolyte Hydrogels to Animal Tissues: A Simple Way to Reseal Cut or Damaged Tissues without Sutures— ***Leah K Borden***, *Srinivasa R. Raghavan*
5:18 Paper 379h: Osmotic-Capillary Principles for Microfluidic Pumping and Fluid Management for Sweat Sensing Devices — ***Tamoghna Saha***, *Jennifer Fang, Sneha Mukherjee, Michael D. Dickey, Orlin Velev*

(380) Interfacial Processes at Biomembranes

Tuesday, Nov 9, 3:30 PM
Sheraton Back Bay, Back Bay Ballroom B

Susan Daniel, Chair
Peter Beltramo, Co-Chair

Sponsored by: Interfacial Phenomena

3:30 Paper 380a: Dilatational Mechanics Evolution of Lung Surfactant Film throughout Acute Respiratory Distress Syndrome Progression Leads to Lung Collapse — ***Clara Ciutara***, *Joseph Zasadzinski*
3:45 Paper 380b: Domain Shape Morphologies in Monolayer Films: Interplay Among Line Tension, Dipolar Repulsions, and Surface Curvature — ***Joseph Barakat***, *Cain Valtierrez-Gaytan, Benjamin Stottrup, Joesph A. Zasadzinski, Todd Squires*
4:00 Paper 380d: The Effect of Headgroup Charge on Symmetric and Asymmetric Phospholipid Bilayers — *Paige Liu, Oscar Zabala-Ferrera,* ***Peter Beltramo***
4:15 Paper 380e: Straining Membrane Vesicles and Cells in Aqueous Nematic Liquid Crystals — ***Purvil Jani***, *Karthik Nayani, Marshall Colville, Matthew Paszek, Nicholas L. Abbott*
4:30 Paper 380f: The Role of Intrinsically Disordered Proteins in Membrane Curvature Sensing — ***Wade Zeno***, *Jeanne C. Stachowiak*
4:45 Paper 380g: The Interplay between Curvature Sensing and Self-Organization of Membrane-Bound Septin Filaments — ***Wenzheng Shi***, *Kevin Cannon, Amy Gladfelter, Ehssan Nazockdast*
5:00 Paper 380h: Gram-Positive Bacterial Membrane Model Developed Using Membrane Vesicles to Study Biophysical Properties and Antibiotic Interactions— ***Samavi Farnush Bint E Naser***, *Zeinab Mohamed, Susan Daniel*
5:15 Paper 380i: Modeling Passive and Active Transport of Antiretroviral Drugs across the Blood Brain Barrier for Treatment of Alzheimer's Disease — ***Daisy Fuchs***, *Kayla Sprenger*
5:30 Paper 380j: Multiway Clustering of Ganglioside GM1 in Heterogeneous Lipid Membranes By Sphingomyelinase-Mediated Hydrolysis — ***Hyun-Ro Lee***, *Siyoung Choi*
5:45 Paper 19h: Interfacial Rheology of Phospholipid Monolayers — ***Damian Renggli***, *Jan Vermant*

(381) Interfacial Transport Phenomena

Tuesday, Nov 9, 3:30 PM
Sheraton Back Bay, Back Bay Ballroom C

Stephen Martin, Chair
Vivek Sharma, Co-Chair

Sponsored by: Interfacial Phenomena

3:30 Paper 381a: Influence of the Immobilization of an Organic Acid in Nafion on Its Microscopic Transport and Structural Properties By Advanced NMR and Small Angle Scattering Techniques — ***Blake Trusty***, *Samuel Berens, Junchuan Fang, Anastasios Angelopoulos, Jonathan Nickels, Sergey Vasenkov*
3:50 Paper 381b: Hydrodynamics of Extended Rods on Curved Fluid Membranes — ***Wenzheng Shi***, *Ehssan Nazockdast*
4:10 Paper 381c: *In Situ* Optical Mapping of Interfacial Mobility and Amphiphile Concentrations at Liquid Crystal-Water Interfaces — ***Sangchul Roh***, *Nicholas L. Abbott*
4:30: Break
4:50 Paper 381g: Simulation of Marangoni Transport from Two Interacting Surfactant Sources — ***Steven Iasella***, *Stephen Garoff, Todd M. Przybycien, Robert D. Tilton*
5:10 Paper 381i: Inertial Spreading and Imbibition on Porous Surfaces in Microgravity — ***Shilpa Sahoo***, *Michel Louge, Olivier Desjardins*
5:30 Paper 381j: Dynamics of Surfactant Spreading on Deep Viscous Films — *Qian Zhang, Carlos Corvalan, Sebastián Ubal,* ***Jiakai Lu***

(382) LGBTQ+ Inclusion in Engineering: Advocating for Minorities

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 204

Gayle Gibson, Co-Chair
Alon McCormick, Co-Chair

Sponsored by: LGBTQ+ and Allies Community

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(383) Mathematical Modeling of Transport Processes

Tuesday, Nov 9, 3:30 PM
Sheraton Back Bay, Republic Ballroom A

Norman Loney, Chair
Dmitry Kopelevich, Co-Chair

Sponsored by: Transport Processes

3:30 Paper 383a: Nonequilibrium Phase Stability of Ion Intercalation Materials—Nonisothermal Effects — ***Debbie Zhuang***, *Dimitrios Fraggedakis, Martin Z. Bazant*
3:51 Paper 383g: Mechanism of Electrohydrodynamic Dispersion of Polyelectrolytes — ***Dmitry Kopelevich***, *Jason Butler*
4:12 Paper 383c: Interfacial Thermal Conductivity and Its Anisotropy — ***Xiaoyu Wang***, *Cynthia J. Jameson, Sohail Murad*
4:33 Paper 383d: Acoustothermal Heating in an Open Microfluidic Channel— ***Pradipta Das***, *Venkat Bhethanabotla*
4:54 Paper 383e: Upscaling of Pore-Scale Simulations — ***Liang Yu***, *Tony Ladd, Piotr Szymczak*
5:15 Paper 383f: Modeling of Mass Transfer of Floral Volatiles across the Plant Cell Wall — ***Meng-Ling Shih***, *John A. Morgan*

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(384) MOF, COF, and Porous Polymer Materials

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 103

Satish Nune, Chair
Ravichandar Baburao, Co-Chair

Sponsored by: Inorganic Materials

3:30 Paper 384a: Understanding Flow Coating Based Large Area MOF Thin Films Formation Using in-Situ Scattering Techniques — ***Gaurav Giri***
4:00 Paper 384b: Mechanistic Study on Thermally-Induced Lattice Stiffening of ZIF-8 — ***Kumar Varoon Agrawal***
4:20 Paper 384c: Correlating Variance in MOF Synthesis with Transport in MOF/Polymer Composites — ***Justin Teesdale***, *Qihui Qian, Zachary Smith*
4:40 Paper 384d: Scalable Routes to Synthesis and Processing of Imine-Linked Cofs — *Dongyang Zhu,* ***Rafael Verduzco***
5:00 Paper 384e: Fabrication of Polyvinyl Alcohol (PVA) - Uio-66 Mixed Matrix Membranes for Water Desalination and Ion-Transport Studies — ***Prince Verma***, *Mara Kuenen, Mark Bannon, Sean Bannon, Geoffrey Geise, Rachel Letteri, Gaurav Giri*
5:20 Paper 384f: Small Molecule Diffusion Studies in High Aspect Ratio, Thin Film, Single Crystalline Metal Organic Frameworks — ***Natalie Smith***, *Gaurav Giri, Nathan Swami*
5:40 Paper 384g: Synthesis and Properties of Metal-Organic Frameworks Containing Lanthanide Clusters — ***Kenneth J. Balkus Jr.***, *Juan Vizuet, Marie Mortensen, Gregory McCandless*

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(385) Nanomaterials for Energy Storage and Conversion 2

Tuesday, Nov 16, 12:30 PM
Virtual, Nanoscale Science and Engineering Forum (22)

Seung Soon Jang, Chair
Ling Fei, Co-Chair
Tae-Sik Oh, Co-Chair

Sponsored by: Nanomaterials for Energy Applications

12:30 Paper 385a: Harmonic Enhancement of Activity and Stability of Iridium-Based Catalysts for Proton Exchange Membrane Water Electrolysis — *Seung Woo Lee, Chaekyung Baik,* ***Chanho Pak***
12:55 Paper 385b: Photocatalytic Core-Shell Nanotube Array Converting Carbon Dioxide and Water to Fuels — ***Won Jun Jo***, *Heinz Frei*
1:15 Paper 385c: Impact of Crystalline Structure on Photodynamics in Halide Perovskites — ***Hyungjun Kim***
1:35 Paper 385d: Phase Transition and Metal Exsolution in Perovskites to Enhance the Catalytic Activity for Hydrogen Production and Conversion — *Kyeounghak Kim, Rui Huang, Chaesung Lim, Hyung Jun Kim,* ***Jeong Woo Han***
1:55 Paper 385e: First-Principles Design on Small Cluster Catalysts for the Electrochemical NH_3 Synthesis By Ligand Engineering — *Seung-hoon Kim, Ho Chang Song, Jonghee Han, Kwan-Young Lee,* ***Hyung Chul Ham***
2:15 Paper 704c: A General Approach to Synthesize Free-Standing Metal Selenides@ Carbon Nanofibers Anode for Lithium/Sodium Ion Batteries— ***Zizhou He***, *Jed LaCoste, Ryan Cook, Ling Fei*
2:35 Paper 140g: Tuning Photocurrent Responses from Photosystem I Interfaced with Tailored Plasmonic Gold and Silver Nanopatterns — ***Ravi Pamu***, *Benjamin Lawrie, Bamin Khomami,* ***Dibyendu Mukherjee***

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(386) Nanoscale Materials-Novel Synthesis Methods and Catalytic Applications

Tuesday, Nov 9, 3:30 PM
Marriott Copley Place, Wellesley

Shohreh Hemmati, Chair
Shu Hu, Co-Chair

Sponsored by: Nanoscale Science and Engineering Forum

3:30: Introductory Remarks
3:48: Break
4:06 Paper 386c: Green Synthesis of One-Dimensional Silver Nanostructures Using Tannic Acid Simultaneously As Reducing, Stabilizing, and Capping Agent-Parametric Study — ***Sina Kaabipour***, *Shohreh Hemmati*
4:24 Paper 386d: Peptide-Mediated Fabrication of Pd−Au Nanocatalysts: Effect of Metal Composition and Catalyst Design Approach on Nitrite Reduction in Water — ***Imann Mosleh, PhD***, *Alireza Abbaspourrad*
4:42 Paper 386e: Colloidal Synthesis of Zinc Tin Phosphide Nanocrystals— ***Ingrid J. Paredes***, *Scott Lee, Matthew W. Greenberg, Sanjit Ghose, Anatoly I. Frenkel, Ayaskanta Sahu*
5:00 Paper 386f: Synthesis of Water-Dispersible $Ti_3C_2T_z$ Mxene Nanosheets By Molten Salt Etching — *Kailash Arole, Miladin Radovic, Jodie Lutkenhaus,****Micah Green***
5:18 Paper 386g: Plasmonic Photocatalysis for Gas-Phase Degradation of Total Volatile Organic Compounds: Theory, Experimentation, and Catalyst Stability— ***Amaury Betancourt***, *D. Yogi Goswami, John Kuhn, Venkat Bhethanabotla*
5:36 Paper 386h: Chiral Self-Assembled Structures of Bowtie Shape: Synthesis, Optical Properties, and Deep Learning-Based Modeling. — ***Anastasiia Visheratina***, *Prashant Kumar, Ji-Young Kim, Alexander Visheratin, Nicholas Kotov*

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(387) New Developments in Computational Catalysis III: Structure-Property Relationships

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 206

Peng Bai, Chair
Florian Goeltl, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

3:30 Paper 387a: A Combined Graph Theory and Machine Learning Based Method for Estimating Complex Adsorbate Configurations on Model Catalytic Surfaces — ***Siddharth Deshpande***, *Pushkar Ghanekar, Jeffrey Greeley*
3:50 Paper 387b: Machine Learning for the Study of Complex Surface Chemistries — *Wenqiang Yang,* ***Andreas Heyden***
4:10 Paper 387c: Simultaneous Screening of Alloy Surfaces for Catalytic Performance and Stability in Reaction Conditions — ***Gloria Sulley***, *Matthew Montemore*
4:30 Paper 387f: Designing Coke-Resistant Dehydrogenation Catalysts with DFT and Grand Canonical Monte Carlo Simulations — ***Peng Wang***, *Thomas Senftle*

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(388) Novel Reactors II (Novel Reactor Configurations)

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 300

Kent J. Warren, Chair
Alan Weimer, Co-Chair
Saurabh Bhandari, Co-Chair

Sponsored by: Process Intensification & Microprocess Engineering

3:30 Paper 388a: Kinetic Model and Autothermal Reactor Design for the Oxidative Dehydrogenation of Ethane — ***Jiakang Chen***, *Praveen Bollini, Vemuri Balakotaiah*
3:50 Paper 388b: Single Reactor Design Concepts for Achieving an Autothermal Operation of Exothermic Oxidative Coupling of Methane and Endothermic Methane Dehydroaromatization Reaction — ***Muhammad Umar Jamil***, *Mamoun Al-Rawashdeh*
4:10 Paper 388c: Effect of Cavitation Intensity on Thermal Efficiency and Reactive Performance of a Hydrodynamic Cavitation Reactor — ***Nasser Al Azri***, *Riddhesh Patel, Hari Mantripragada, Robert M. Enick, Goetz Veser*
4:30 Paper 388d: Continuous Biphasic Microreactor for Production of Hydrogen Peroxide Via Non-Thermal Atmospheric Pressure Plasma — ***Fabio Cameli***, *Tai-Ying Chen, Panagiotis Dimitrakellis, Dionisios Vlachos*
4:50 Paper 388e: Zero-D Thermodynamic Model As a Simple Tool for Screening Chemical Reaction Candidates and Benchmarking of the Piston Reactor Technology — ***Aya Abousrafa***, *Mamoun Al-Rawashdeh*
5:10 Paper 388f: Modeling a Fluidized Bed Reactor for Particle Atomic Layer Deposition with CFD-DEM — ***Davis Conklin***, *Julia Hartig, Alan Weimer*

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(390) Photovoltaic, Thermoelectric, and Energy Materials

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 104

Charles Hages, Chair

Sponsored by: Electronics and Photonics

3:30 Paper 390a: Controlling Crystallization for Large Ligand Incorporation into Quasi-2D Perovskite Solar Cells — ***Aidan Coffey***, *Letian Dou*
3:45 Paper 390b: Evaluation of Life Cycle Environmental Impacts of Chemical Precursors Used in Perovskite Photovoltaics Manufacturing. — ***Sherif Khalifa***, *Sabrina Spatari, Aaron T. Fafarman, Jason Baxter*
4:00 Paper 390c: Direct Solution Deposition of Metal Selenide Semiconductors Using Novel Metal-Selenium Complexes — ***Jonathan Turnley***, *Swapnil Dattatray Deshmukh, Rakesh Agrawal*
4:15 Paper 390d: Double Cation Substitution of CZTS Chalcogenide Semiconductors for Improved Device Performance — ***Jeffrey Chin***
4:30 Paper 390e: Optoelectronic Characterization of Silver-Doped Cu_3AsS_4 for Photovoltaic Applications — ***Apurva Pradhan***, *Kyle Weideman, Rakesh Agrawal*

4:45 Paper 390f: Deeply Rechargeable Zinc Anode Materials for Ultra-Safe High-Energy Rechargeable Batteries — ***Nian Liu***
5:00 Paper 390g: Ni-Fe Layered Double Hydroxides and Ni-Sulfide Electrocatalyst Foams for Electrochemical Energy Storage and Conversion Devices — ***Enoch Nagelli***, *Caspar Yi, F. John Burpo, Sean P. Rogers, Matthew A. Dibiase, Jiangtian Li, Rongzhong Jiang, Deryn Chu*

(391) Plenary Session: Waste Plastics (Invited Talks)

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 200

Jeffrey Seay, Chair

Sponsored by: Waste Plastics

3:30 Paper 391a: Alliance to End Plastic Waste: Global Activities in Combating Plastics Waste — ***Joseph Machado***, *Elesia Glover*
4:00 Paper 391b: Eastman in the Circular Economy – How Life Cycle Assessment (LCA) Enables Commercial Scale Molecular Recycling — ***Teni Butler***
4:30: Break
5:00 Paper 391d: Creating a Pure Planet by Transforming Recycling — ***Dustin Olson***

(392) Polymers in Additive Manufacturing

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 202

Blair Brettmann, Chair
Michael Bortner, Co-Chair

Sponsored by: 3D Printing

3:30 Paper 392a: High Strength, High Toughness Parts Via Dual Material Fused Filament Fabrication — *Brian Koker, Rebecca Ruckdashel, Hikma Abajorga, Ryan Dunn, David Kazmer, Eric D. Wetzel,* ***Jay Park***
3:55 Paper 392b: Process-Structure-Property Relationships in Additively Manufactured Polypropylene Blends — ***Arit Das***, *Michael Bortner*
4:20 Paper 392c: Understanding Flow and Stress Development in 3D Printing By Material Extrusion — ***Bryan Vogt***
4:45 Paper 392d: Autonomic Self-Healing of 3D Printed Polymer Composites— ***Vinita Shinde***, *Asha-Dee Celestine, Lauren Beckingham, Bryan Beckingham*
5:10 Paper 392e: Synthesis, Characterization, and Application of Novel Surface-Eroding Photopolymer Formulations — ***Whytneigh Duffie***, *Kevin D. Barz, Tsvetanka S. Filipova, Timothy M. Brenza, Katrina J. Donovan, Travis W. Walker*
5:35 Paper 392f: Designing New Printable Thermoset Shape Memory Polymers Via Molecular Simulation and Machine Learning — ***Andrew Peters***, *Anwar Shafe, Aniruddha Chowdhury, Guoqiang Li, Collin D. Wick*

(393) Polymer Thin Films, Confinement, and Interfaces II

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 107

Rong Yang, Chair
Stephen Martin, Co-Chair
Kathleen McEnnis, Co-Chair
Caroline Szczepanski, Co-Chair

Sponsored by: Polymers

3:30 Paper 393a: Understanding the Modification of Local Glass Transition Dynamics By Surface Bound Chains — ***Connie Roth***
4:00 Paper 393c: High Throughput Screening Test for Adhesion in Polymer Films Using Centrifugation — *Yusu Chen, Qifeng Wang, Carolyn E. Mills, Johanna G. Kann, Kenneth R. Shull, Danielle Tullman-Ercek,* ***Muzhou Wang***
4:15 Paper 393d: Fine Tuning the Interaction Parameter for Sub-10 Nm Block Copolymer Directed Self-Assembly — ***Whitney Loo***, *Hongbo Feng, Ricardo Ruiz, Paul F. Nealey*
4:30 Paper 393e: Light-Mediated Polymerization for the Engineering of Advanced Surfaces — *Michele Fromel, Dhanesh Ranaweera,* ***Christian Pester***, *Devon Sweeder, Mingxiao Li*
4:45 Paper 393f: Vapor Deposition of Microstructured Silicon-Containing Polymer Films on High Viscosity Silicone Oils — ***Nicholas Welchert***, *Bryan Nguyen, Malancha Gupta, Theodore T. Tsotsis*
5:00 Paper 393g: Template-Free Alignment of Lamellar Block Copolymers for Large Area Sub-10 Nm Patterning — ***Maninderjeet Singh***, *Chenhui Zhu, Joseph Strzalka, Jack F. Douglas, Alamgir Karim*
5:15 Paper 393h: Polymer Dynamics in Disordered Nanoparticle Packings— ***Bharath Venkatesh***, *Daeyeon Lee*
5:30 Paper 393b: Versatile Polymer Nanoparticle Synthesis Using Initiated Chemical Vapor Deposition (iCVD) — ***Trevor Donadt***, *Danielle Streever, Rong Yang*

(394) Process Intensification and Modular Manufacturing: Chemical Commodity Processes

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 209

Fereshteh Farzad, Chair
Ignasi Palou Rivera, Co-Chair

Sponsored by: Process Intensification & Modular Chemical Processing

3:30 Paper 394a: Advances in Absorbent-Enhanced Ammonia Production— ***Matthew Palys***, *Mitchell Hockenberry, Emmanuel Onuoha, Alon McCormick, Prodromos Daoutidis*
3:50 Paper 394b: Process Intensification for Olefins Recovery — ***Hannah Murnen***, *Christine Parrish, William Charlton, Sudip Majumdar*
4:10 Paper 394c: Residence Time Distribution Studies of a Hydrodynamic Cavitation Reactor — ***Riddhesh Patel***, *Nasser Al Azri, Hari Mantripragada, Robert M. Enick, Goetz Veser*
4:30 Paper 394d: Process Intensification Via Thin Film Evaporation for Simultaneous Reaction and Separation in Dispersants Production — ***Hari Mantripragada***, *Nasser Al Azri, Riddhesh Patel, Robert M. Enick, Goetz Veser*

(395) Reaction Chemistry and Engineering II

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 207

Andrew R Teixeira, Chair
Pranav Karanjkar, Co-Chair
Pranit S. Metkar, Co-Chair
Joshua Allen, Co-Chair
Milad Abolhasani, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

3:30 Paper 395a: Direct Methylation of Cobaloxime By Low Temperature Methane Plasma in a Multiphase DBD μ-Plasmatron — *Yukun Liu,* ***Ryan Hartman***
3:48 Paper 395b: Co-Hydrothermal Carbonization (Co-HTC) of Biomass-Plastic Blend: Enhancement of Fuel Quality — ***Md Tahmid Islam***, *Nepu Saha, Jordan Klinger, Toufiq Reza*
4:06 Paper 395c: Solvothermal Liquefaction of Mixed Waste Plastics: Effect of Solvents at Sub-and Supercritical Conditions — ***Soudeh Banivaheb***, *Nepu Saha, Toufiq Reza*
4:24 Paper 395e: Selective Ring Opening of Decalin over Ion-Exchanged Ir Zeolites — ***Matthew J. Kline***, *Sampath A. Karunarathne, Thomas Schwartz, Clayton Wheeler*
4:42 Paper 509ch: Forced Thermal Oscillations in Catalytic Microreactors— ***Cameron Armstrong***, *Andrew R Teixeira*
5:00 Paper 395g: Nickel-Iron Catalysts for Low Temperature Dry Reforming of Methane — ***Gagandeep Dhillon***, *Nan Yi*
5:18: Break

(396) Remediation of Emerging Contaminants and Legacy Compounds II

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 308

Sage Hiibel, Chair
Robert Peters, Co-Chair
Alexander Dowling, Co-Chair

Sponsored by: Water

3:30 Paper 396a: Thermally Enhanced Advanced Oxidation-Driven Regeneration on Iron-Activated Biochar for Removal of Microcystin-LR in Water and Wastewater — *Shengquan Zeng,* ***Eunsung Kan***
3:55 Paper 396c: Reversible Adsorption and Desorption of Pfas Via Switching the Electric Field on Carbonaceous Adsorbents — ***Bishwash Shrestha***, *Mohammadamin Ezazi, Sanjay Ajayan, Gibum Kwon*
4:20 Paper 396d: Investigating Lead Biosorption Mechanisms at Trace Concentrations — ***Patritsia Stathatou***, *Christos E. Athanasiou, Andreas Mershin, Marios Tsezos, Neil Gershenfeld*
4:45 Paper 396e: Micelle-Laden Hydrogel Microparticles for the Removal of Hydrophobic Micropollutants — ***Devashish Gokhale***, *Patrick S. Doyle*
5:10 Paper 396f: Adsorption and on-Demand Desorption of Perfluoroalkyl Substances in Water By Thermo-Responsive Poly(N-isopropylmethacrylamide)— ***Mohammadamin Ezazi***, *Bishwash Shrestha, Eden Surafel Taddese, Gibum Kwon*

(397) Renewable Fuels Production from Hydrogen and Captured CO_2 or N_2

Thursday, Nov 18, 12:30 PM
Virtual, Synthetic & Renewable Fuels (TH)

Eric Miller, Chair
William Gibbons, Co-Chair

Sponsored by: Synthetic & Renewable Fuels

12:30 Paper 397a: An Electrofuel Revolution: How Direct Carbon Reduction Can Electrify the Future — ***Michael Orella***, *Achim Wechsung, Michael Stern, Harri Kytomaa*
12:45 Paper 397b: Engineering Yeast to Synthesize Semiconductor Nanoparticles Allowing Light Driven CO_2 Fixation and Biofuel Production— ***Shalmalee Pandit***, *Zhaoqi Li, George Sun, Matthew Vander Heiden, Angela M. Belcher*
1:00 Paper 397c: Direct Conversion of Industrial Exhaust Gas to a C40 Natural Product By Biologic/Inorganic Hybrid Catalysis — ***Haoliang Wu***, *Haojie Pan, Zhongjian Li, Jiazhang Lian*
1:15 Paper 397d: A Comparative Assessment Framework for Sustainable Production of Fuels and Chemicals Explicitly Accounting for Intermittency— ***Caroline Ganzer***, *Niall Mac Dowell*
1:30 Paper 397e: Cheap Energy Is a Key to Competitive Artificial Fuels— ***David Judbarovski***

(398) Soft and Active Systems

Tuesday, Nov 9, 3:30 PM
Sheraton Back Bay, Constitution A

Sujit Datta, Co-Chair
John Berezney, Co-Chair

Sponsored by: Fluid Mechanics

3:30 Paper 398a: Life in a Tight Spot: How Bacteria Swim, Disperse, and Grow in Complex

Spaces — *Tapomoy Bhattacharjee, Daniel B. Amchin, Jenna Ott, Ricard Alert, Felix Kratz,* ***Sujit Datta***
3:45 Paper 398b: Phoretic Motion in Active Matter — ***John Brady***
4:00: Break
4:15 Paper 398d: Enhanced Bacterial Motility in Complex Fluids — ***Shashank Kamdar****, Seunghwan Shin, Xinliang Xu, Lorraine F. Francis, Xiang Cheng*
4:30 Paper 398e: Bacteria As Active Colloids on Fluid Interfaces — ***Jiayi Deng****, Mehdi Molaei, Nicholas Chisholm, Kathleen J. Stebe*
4:45 Paper 398f: Coil-Stretch-like Transition and Wrinkling Dynamics of Elastic Sheets in Extensional Flows — ***Yijiang Yu****, Michael Graham*
5:00 Paper 398g: Self-Propulsion of a Freely Suspended Swimmer By a Swirling Tail in a Viscoelastic Fluid — ***Jeremy Binagia****, Eric Shaqfeh*
5:15 Paper 398h: Viscoelasticity Encodes Longevity of Transient Dynamical States in Active Fluids — ***John Berezney****, Seth Fraden, Zvonimir Dogic*
5:30 Paper 398i: Gaussian-Curvature-Mediated Interactions of Elastic Inclusions in Fluid Membranes — ***Joseph Barakat****, Todd Squires*

(400) Technology Transfer and Industrial-Academic Interfaces

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 203

Joshua Schaidle, Chair
Sarika Goel, Co-Chair
Brandon O'Neill, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

3:30 Paper 400a: Carbon Capture Technology and Natural Gas Treatment— ***Margaret Greene****, Justin Pan, Brian Houston*
3:48 Paper 400b: From Discovery to Deployment of an Aromatic Transalkylation Catalyst — ***Christina Elia****, Joshua Cutler, Joseph E. Gatt, Anna Ivashko, Kathy Keville, Frank Lai, Brett Loveless, Michel Molinier, Hari Nair, Nicholas Rollman, Bob Tinger, Dominick Zurlo*
4:06 Paper 400c: Integrated Capture and Conversion of CO_2 into Materials (IC^3M); A Multi-Product Technology for Ccus — *Jotheeswari Kothandaraman, Johnny Saavedra-Lopez, Yuan Jiang, Robert A. Dagle,* ***David Heldebrant***
4:24 Paper 400d: Developing Biomass Valorization Technologies Based on Functionalization Chemistry — ***Jeremy Luterbacher***
4:42 Paper 400e: Heavy Oil Reforming in a Dual Circulating Fluidized Bed Reactor — ***Girish Srinivas****, Steve Schwab, Steven Gebhard*
5:00 Paper 400f: Catalyst Development and Process Intensification of a Bio-Renewable Surfactants Platform — *Cameron Moore,* ***Xiaokun Yang****, Troy Semelsberger, Shawn Eady, Christoph Krumm*
5:18 Paper 400g: Test Tubes to Tons: De-Risking Pyran's Novel Catalytic Pathway to Bio-Based 1,5-Pentanediol — *Daniel J. McClelland, Nikhil Victor, George Huber,* ***Kevin Barnett***
5:36 Paper 400h: Technology Transfer for Producing Sustainable Aviation Fuels from Wet Waste — ***Derek Vardon***

(401) Tools and Techniques for Sustainable/Green Product Design

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 303

Mrunmayi Kumbhalkar, Chair
Shaibal Roy, Co-Chair
Sitaraman Krishnan, Co-Chair

Sponsored by: Product Design

3:30: Introductory Remarks
3:35 Paper 401c: Enhancing the Dielectric Breakdown Strength of Solid-State Polymer Capacitors By Chain End Manipulations — ***Maninderjeet Singh****, Saumil Samant, Mei Dong, David Tran, Nihar Pradhan, Dharamraj Raghavan, Karen Wooley, Alamgir Karim*
3:55 Paper 401e: Electropolymerization of Polypyrrole By Photosystem I— ***Joshua Passantino****, Inaya Molina, David Cliffel, G. Kane Jennings*
4:15 Paper 401g: Development of Electrically Reversible Ion Exchange (ERIE) Electrodes for Desalination and Aqueous Deionization — ***Michael Mullins****, Janet Metsa*
4:35 Paper 401i: A Multi-Scale Approach to Evaluate the Relationship between Rheological and Textural Properties of Oil-in-Water Cosmetic Emulsions— ***Fernando Calvo****, Ingrid Gomez, Jorge M. Gomez, Luis Ricardez-Sandoval, Oscar Alvarez*
4:55 Paper 401d: Cyclic Carbonate Plasticizers to Improve Li-Ion Conductivity in Solid Polymer Electrolytes — ***Anthony Engler****, Habin Park, Emily Brooks, Nian Liu, Paul A. Kohl*
5:15 Paper 401f: Design and Application of Hydrophobic 2,2,4-Trimethyl-1,3-Pentandiol Deep Eutectic Solvents for Boron Extraction — *Narjis Awaja,* ***Ghaiath Almustafa****, Ahmad S. Darwish, Ioannis Zuburtikudis, Hadil AbuKhalifeh, Hassan Arafat, Inas AlNashef*

(402) Topical Plenary: Antimicrobial Platforms and Materials Addressing Current Health Challenges (Invited Talks)

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 310

Tagbo H. R. Niepa, PhD, Chair
Nuno F. Azevedo, Co-Chair
Sricharani Balmuri, Co-Chair

Sponsored by: Microbes at Biomedical Interfaces

3:30 Paper 402a: Invited Talk: Machine Biology for Infectious Diseases— ***Cesar de la Fuente-Nunez***
4:00 Paper 402b: Invited Talk: Nucleic Acid Mimics-Based Strategies to Tackle Antimicrobial Resistance in Bacteria — ***Nuno Azevedo***
4:30 Paper 402c: Invited Talk: The Biofilm Matrix As a Therapeutic Target— ***Kendra Rumbaugh***
5:00 Paper 402d: Invited Talk: Probing Bacterial Social Behaviors during Human Infection — ***Marvin Whiteley***
5:30 Paper 402e: Invited Talk: Harnessing Synthetic Biology to Characterize and Treat the Gut Microbiome — ***James J. Collins***

(403) Water Treatment, Desalination, and Reuse III

Tuesday, Nov 9, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 312

Alexander Lopez, Co-Chair
Milad Esfahani, Co-Chair

Sponsored by: Membrane-Based Separations

3:30 Paper 403a: Pressure-Controlled Nanochannels in Polymer Cross-Linked Graphene Oxide Membranes for Water Treatment: A Combined Experimental – Molecular Simulation Approach — ***Daniel Bahamon****, Ki Ryuk Bang, Eun Seon Cho, Lourdes F. Vega*
3:51 Paper 403c: Functionalized-Mxene Thin Film Nanocomposite Membranes for Removal of Polyfluoroakyl Substances from Water — ***Tin Le****, Milad Esfahani*
4:12 Paper 403d: Atomic Layer Deposition-Modified Membranes for Produced Water Treatment — ***Diako Mahmodi****, Anil Ronte, Seokjhin Kim, Joshua Ramsey*
4:33 Paper 403e: Molecular Simulations of POC/Sbad-1 Mixed-Matrix Membranes for Water Desalination — ***Lin Li****,* ***Jie Liu***
4:54 Paper 403f: Scaleup of Membrane Distillation for Desalination of Produced Water from Unconventional Reservoirs. — ***Ritesh Dinkar Pawar****, Zhewei Zhang, Radisav Vidic*
5:15 Paper 403g: Modeling of Solute-Coupled Transport in Osmotically-Assisted Membrane Separations with Multicomponent Solution-Diffusion Theory— ***Zi Hao Foo****, Danyal Rehman, Orisa Coombs, Akshay Deshmukh, John Lienhard*
5:36 Paper 408a: High-capacity adsorbents with hierarchical structures printed from polymer composites — *Jialing Xu, Thomas Kasl, Adam Braegelman, Kevin Gabriel Alvarez, Matthew Webber,* ***William Phillip***

(404) D.I.C. Wang Award Lecture

Tuesday, Nov 9, 6:15 PM
John B. Hynes Veterans Memorial Convention Center, 302

Sponsored by: Awards Committee

6:15 Paper 404a: Exploiting Redox for Connecting Biology to Electronics – Controlling Behavior via Electrogenetics — ***William Bentley***

(405) Academic Ableism and Education

Monday, Nov 15, 8:00 AM
Virtual, Engineering for Inclusion (TC)

Christopher Pope, Chair
Melissa A. Postlewaite, Co-Chair
De-Wei Yin, Co-Chair

Sponsored by: Disabilities OutReach & Inclusion Community (DORIC)

(407) Advanced Biomass Conversion Technologies

Wednesday, Nov 10, 8:00 AM
Marriott Copley Place, Provincetown

Xinshu Zhuang, Chair
Shijie Liu, Co-Chair

Sponsored by: Forest and Plant Bioproducts Division

8:00 Paper 407a: Could Benzyl Hydroxyl Shielding Promote the Radical Induced Pyrolysis of Lignin? — ***Yuyang Fan****, Ming Lei, Chao Liu, Rui Xiao*
8:15 Paper 59a: Decarbonising the UK Heating Sector: A Whole-Energy System Analysis — *Matthias Mersch,* ***Nixon Sunny****, Christos N. Markides, Niall Mac Dowell*
8:30 Paper 407c: Techno-Economic Assessment of Three Potential Pathways for Biomass Liquefaction — ***Akash Kailas Patil****, Pahola Thathiana Benavides, Dale Monceaux, Abigail Engelberth*
8:45 Paper 407d: Valorization of Pear Pomace: Composting and Reusing on Site — *Facundo Iturmendi, N. Bongiovani, Juan Ignacio Laiglecia, R. Hollzman,* ***Patricia Hoch***
9:00 Paper 407e: Altering Physico-Chemical Properties of Pine-Derived Carbon Quantum Dots By Changing Hydrothermal Treatment Conditions — ***Thomas Quaid****, Toufiq Reza*
9:15 Paper 407f: Understanding the Effects of Mixed Municipal Solid Waste Streams on HTL Product Characteristics — ***Heather O. LeClerc****, Michael T. Timko, Andrew R Teixeira*
9:30 Paper 407g: Adsorption Kinetics Studies of Catalytic HTL Derived Biochar— ***Khang Huynh****, Bharath Maddipudi, Vinod Amar, Anuradha Shende,* ***Rajesh Shende***

(409) Bionanotechnology for Drug Delivery

Wednesday, Nov 10, 8:00 AM
Marriott Copley Place, Simmons

Joo-Youp Lee, Co-Chair
Aaron Anselmo, Co-Chair

Sponsored by: Bionanotechnology

8:00 Paper 409a: Aerosol Nanocomposite Systems Comprised of Cell Membrane-Coated Nanoparticles for the Treatment of Pulmonary Diseases— ***Samantha Meenach****, Md Golam Jakaria*
8:25 Paper 409b: Effect of Drug Hydrophobicity on X-Ray-Triggered Drug Release from Peg-PLA/$CaWO_4$ Nanoparticles: A Study of Stereoisomers of

paclitaxel — ***Kaustabh Sarkar***, *Sandra Torregrossa-Allen, Melanie Currie, Mark Langer, Gregory Durm, Bennett D. Elzey, Sanjeev Narayanan, You-Yeon Won*
8:50: Break
9:15: Break
9:25 Paper 409f: Liposome and Polyelectrolyte Layers Derived Single Shot Vaccine Platform for Controlled Release of Inactivated Chikungunya Virus— ***Rashi Porwal***, *Anuj Sharma, Srivatsan Kidambi*
9:50 Paper 409g: Polyethylene Glycol Camouflaged *Lumbricus Terrestris* mega-Hemoglobin for Diverse Oxygen Therapeutic Applications — ***Chintan Savla***, *Andre Palmer*

(410) Carbon Nanomaterials: Adsorption, Separations, and Transport Processes

Wednesday, Nov 10, 8:00 AM
Marriott Copley Place, Wellesley

Christopher Sims, Chair
Kevin Hinkle, Co-Chair
Shohreh Hemmati, Co-Chair

Sponsored by: Carbon Nanomaterials

8:00 Paper 410b: Separations and Measurements of Single-Wall Carbon Nanotube Enantiomers — *Christopher Sims, Han Li, Benjamin Flavel,* ***Jeffrey Fagan***
8:25 Paper 410c: A Spin-Coated Hydrogel Platform Enables Accurate Investigation of Immobilized Individual Single-Walled Carbon Nanotubes— ***Matthew Card***, *Mitchell Gravely, Seyedeh Zahra Moafi Madani, Daniel Roxbury*
8:50 Paper 410d: Diffusive Heat Transfer in Isolated, Free-Standing, Single-Walled Carbon Nanotubes — ***Matthias Kuehne***, *Samuel Faucher, Zhe Yuan, Michael S. Strano*
9:15 Paper 410e: Controlled Release from Intercalated Graphene Oxide Films: Edge and Basal-Plane-Specific Kinetics of Planar, 1D Wrinkled, and 2D Crumpled Nanochannels — *Muchun Liu,* ***Deisy Cristina Carvalho Fernandes***, *Zachary Saleeba, Robert Hurt*
9:40 Paper 410f: Nanoporous Atomically Thin Graphene Membranes — ***Piran Kidambi***

(411) Catalyst Design, Synthesis, and Characterization I - Characterization and Spectroscopic Studies

Wednesday, Nov 10, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 205

Matteo Cargnello, Chair
Steven Saunders, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

8:00 Paper 411a: Quantitative in-Situ FTIR Analysis of Ce^{3+} Densities and the Role of Oxygen Vacancies in Catalysis over Ceria Surfaces — ***Sadia Afrin***, *Praveen Bollini*
8:20 Paper 411b: Acidity Trends in SiO_2 Overcoated Oxides — ***Andrew Wolek***, *Justin Notestein*
8:40 Paper 411c: Investigating the Redox Behavior of MoOx Catalysts Supported on CeO_2-TiO_2 Via in-Situ Raman and FTIR Spectrokinetics — ***Thu D. Nguyen***, *Fuat E. Celik, George Tsilomelekis*
9:00 Paper 411d: Characterization of Supported Subnanometer Clusters Via Computational Infrared Spectroscopy — ***Vinson Liao***, *Yifan Wang, Maximilian Cohen, Dionisios Vlachos*
9:20 Paper 411e: Low-Temperature Activity and Initiation in Silica-Supported Mo Olefin Metathesis Catalysts — ***Zachariah Berkson***, *Gregory Price, Glenn Sunley, Christophe Copéret*
9:40 Paper 411f: Effects of Reduction Temperature on Negatively Charged Gold Species over Nonreducible Supports — ***Anhua Dong***, *John R. Regalbuto, Christopher Williams*
10:00 Paper 53e: Development of *in Situ* Monitoring of Biomass Reactions Via Spectroscopic Techniques — ***Jakub Konkol***, *George Tsilomelekis*

(413) Computational and Experimental Studies on Protein Structure, Function, and Developability

Wednesday, Nov 10, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 111

Phanourios Tamamis, Chair
Jamie Spangler, Co-Chair

Sponsored by: Bioengineering

8:00 Paper 413a: Molecular Dynamics Simulation on Human β Defensin Type 3 Binding with the CXCR4 Receptor — ***Jackson Penfield***, *Liqun Zhang*
8:18 Paper 413b: Protein Engineering to Improve the Function of BicA: A Constitutively Expressed, High-Flux Bicarbonate Transporter in *Synechococcus*sp. PCC 7002 — ***Sydney Parrish***, *Guanhong Bu, Christopher Jones, David Nielsen, Brent L. Nannenga*
8:36 Paper 413d: Computational Docking and Design of Fixed-Backbone Binding Protein Scaffolds for Target Epitopes — ***Varun Chauhan***, *Robert Pantazes*
8:54 Paper 413e: Calculation of Therapeutic Antibody Viscosity with Computer Simulations — ***Pin-Kuang Lai***
9:12 Paper 413g: TBD Speaker — ***William Schief***

(414) CO_2 Industrial, Engineering and R&D Approaches I

Monday, Nov 15, 8:00 AM
Virtual, Environmental Division (09)

Selen Cremaschi, Chair
Adam Usadi, Co-Chair
Xiaonan Wang, Co-Chair

Sponsored by: Sustainability

8:00 Paper 414a: Pathways for UK Power and Industry to Net-Zero — ***Caroline Ganzer***, *Niall Mac Dowell*
8:15 Paper 414b: Towards a Circular Chemical Industry: Mapping the Flow of Fossil Carbon through Chemical Manufacturing Processes — ***Amrita Sen***, *George Stephanopoulos, Bhavik Bakshi*
8:30 Paper 414c: The Role and Value of Disruptive CCS Technologies for Electricity Systems — ***Yoga Wienda Pratama***, *Niall Mac Dowell*
8:45 Paper 414d: H_2 Roadmap Alternatives for Decarbonizing Singapore through 2050 — *Xiaodong Hong,* ***Iftekhar Karimi***, *Farooq Shamsuzzaman, Xiaonan Wang, Adam Usadi, Bryan R. Chapman, Robert A. Johnson*
9:00 Paper 414e: Packed Bed Column Adsorption and Parametric Analysis of CO2 Onto Palm Kernel Shell Activated Carbon Using Computational Modelling Approach. — ***Abdulfatai Faro***, *Kazeem Salam, Edith Alagbe*
9:15 Paper 414f: Dynamic Modeling and Soft Sensor Based Predictive Control of a Moving Bed Process for CO_2 Capture Using a Micro-Encapsulated Solvent— ***Goutham Kotamreddy***, *Ryan Hughes, Debangsu Bhattacharyya, Benjamin P. Omell, Michael S. Matuszewski*
9:30 Paper 414g: Evaluation of Real Time Optimization – Model Predictive Control and Economic Model Predictive Control Strategies for Post Combustion CCS Operations within Refineries — ***Adhish Chandra Saketh Madugula***, *Tracy Benson*

(415) Data-Driven and Hybrid Modeling for Decision Making I

Wednesday, Nov 10, 8:00 AM
Sheraton Back Bay, Independence Ballroom East

Burcu Beykal, Chair
Zuo Zeng, Co-Chair

Sponsored by: Information Management and Intelligent Systems

8:00 Paper 415a: Modeling Complex Nonlinear Systems Using Concatenated Static-Dynamic Neural Networks — ***Angan Mukherjee***, *Debangsu Bhattacharyya*
8:15 Paper 415b: Optimal Synthesis and Heat Integration Using Generalized Disjunctive Programming with Hybrid Models — *Alejandro Pedrozo Sr., Sabrina Belen Rodriguez Reartes, David E. Bernal, Aldo Vecchietti,* ***Maria Diaz***, *Ignacio Grossmann*
8:30 Paper 415c: Regularized Subsets: A Framework for High-Dimensional Linear Regression with Noisy Data and Optional Constraints — ***Owais Sarwar***, *Nick Sahinidis*
8:45 Paper 415d: A Data-Driven Inverse Optimization Approach to Learning Surrogate Optimizers — ***Rishabh Gupta***, *Qi Zhang*
9:00 Paper 415e: A Hybrid Model Feature Relevance Analysis for Mechanistic Model Refinement Suggestions — ***Yushi Deng***, *Selen Cremaschi, Mario Eden, Haijing Gao, Shuxing Cheng*
9:15 Paper 415f: A General Strategy for Quantification of the Uncertainty on a Hybrid Model's Uncertainty Estimates — ***Francesco Rossi***, *Yan-Shu Huang, Sumit Kumar, Rexonni Lagare, Linas Mockus, Gintaras V. Reklaitis*
9:30 Paper 415g: Machine Learning and Multi-Way Method Modelling Methods for Pharmaceutical Process Quality — ***Atli Magnússon***, *Gürkan Sin, Jari Pajander, Stuart Michael Stocks*
9:45 Paper 415h: Surrogate Thermodynamics for Process Synthesis: A Computational Study on Model Selection, Accuracy and Performance — ***Ashfaq Iftakher***, *Mohammed Sadaf Monjur, Chinmay Aras, M M Faruque Hasan*

(416) Department Heads Forum (Invited Talks)

Wednesday, Nov 10, 8:00 AM
Sheraton Back Bay, Liberty B/C

Daniel F. Shantz, Chair
Clifford L. Henderson, Co-Chair

Sponsored by: Department Heads Forum

8:00: Introductions: Cliff Henderson, University of South Florida, and Dan Shantz, Tulane University
8:10 Paper 416a: Salary Survey — ***Tyler Johannes***
8:40 Paper 416b: ABET Update — ***Randy Lewis***
8:55: Break
9:00 Paper 416c: Department Heads Survey Readout and Discussion— ***Clifford L. Henderson***, *Daniel F. Shantz*
9:30 Paper 416d: State of the Institute — ***June Wispelwey***
10:00: Discussion

(417) Design and Operations Under Uncertainty

Wednesday, Nov 10, 8:00 AM
Sheraton Back Bay, Independence Ballroom West

Dinesh Krishnamoorthy, Co-Chair
Francesco Rossi, Co-Chair

Sponsored by: Systems and Process Operations

8:00 Paper 417a: Nested Sampling Algorithm for Probabilistic Design Space Definition with Recourse Action — ***Kennedy Kusumo***, ***Cornel Marck***, *Nilay Shah,* ***Benoit Chachuat***
8:19 Paper 417b: Rare-Event Sampling for Efficient Scenario Generation for Stochastic Programs — ***David Young***, *Mark Carpenter, Selen Cremaschi*
8:38 Paper 417c: Design Centering through Derivative-Free Optimization — ***Fei Zhao***, *Ignacio Grossmann, Salvador Garcia-Munoz, Stephen D. Stamatis*
8:57 Paper 417d: Random Field Optimization — ***Joshua Pulsipher***, *Victor M. Zavala*
9:16 Paper 417e: Assessing the Demand Response Potential of Power-Intensive Processes By Stochastic Scheduling Optimization — ***Sonja Germscheid***, *Manuel Dahmen, Alexander Mitsos*
9:35 Paper 417f: Accounting for Uncertainty in Production Scheduling in the Presence of Feedback:

Method Comparison, Paradoxes, and Guidelines— ***Venkatachalam Avadiappan***, *Christos Maravelias*
9:54 Paper 417g: Data-Driven Sample Average Approximation with Covariate Information — ***Rohit Kannan***, *Güzin Bayraksan, James Luedtke*

(418) Design and Optimization of Integrated Energy Systems

Wednesday, Nov 10, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 308

Alexander Dowling, Chair
Dhabia Al-Mohannadi, Co-Chair
David Miller, Co-Chair

Sponsored by: Climate Change

8:00 Paper 418a: An Optimization-Based Decision Framework for Integrating Energy Storage with Fossil Power Plants — ***Manali S. Zantye***, *Mengdi Li, Akhilesh Gandhi, Yifan Wang, Sai Pushpitha Vudata, Pavitra Senthamilselvan Sengalani, Debangsu Bhattacharyya, M M Faruque Hasan*
8:15 Paper 418b: Optimization of a Hybrid Biomass and Gas to Liquids Process Via Fischer–Tropsch Synthesis with Integrated Product Refining — ***Yufei Zhao***, *Cornelius Masuku*
8:30 Paper 418c: An Optimization Based Framework for the Design of Biofuels/Fossil Fuels Blendstocks — ***Juan Manuel Restrepo-Florez***, *David Rothamer, Christos Maravelias*
8:45 Paper 418d: Assessment and Optimization of the Economic and Carbon Sequestration Potential of Renewable Energy and Negative Emission Technologies — ***Lanyu Li***, *Xiaonan Wang*
9:00 Paper 418e: Toward Future Energy Generation Systems: Multi-Scale Optimization with Market Interactions — *Jordan Jalving, Jaffer Ghouse, Bernard Knueven, John Siirola,* ***Alexander Dowling***, *David Miller*
9:15 Paper 418f: *The Potential Role and Value of Power-to-Gas Storage in the UK Energy System* — *Caroline Ganzer, Niall Mac Dowell,* ***Yoga Wienda Pratama***

(419) Diffusion, Transport and Dynamics in Adsorption Systems

Wednesday, Nov 10, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 300

Joshua Thompson, Chair
James A. Ritter, Co-Chair

Sponsored by: Adsorption and Ion Exchange

8:00 Paper 419a: Dynamics of Reversible Nanofluidic Water Filling inside Isolated Single-Walled Carbon Nanotubes — ***Samuel Faucher***, *Matthias Kuehne, Michael S. Strano*
8:15 Paper 419b: Evidence of Combined Heat Transfer and Surface Barrier Resistances for Propane in Commercial ZIF-8 Crystals Probed By Pressure-Swing Frequency Response — ***Yu Wang***
8:30 Paper 419c: The Diffusion of CO_2 and N_2 in 13X Zeolite Particles of Different Sizes Using a 100 Hz Volumetric Frequency Response System— ***Armin Ebner***, *James A. Ritter, Charles E. Holland*
8:45 Paper 419d: Diffusion of Pure and Mixed Light Gases in a Commercial 5A Zeolite By High Field NMR Diffusometry — ***Amineh Baniani***, *Yu Wang, Pavel Kortunov, Sergey Vasenkov*
9:00 Paper 419e: Boundary Layer Theory in Fixed-Bed Adsorption — ***Robert DeJaco***, *Anthony J. Kearsley, Paul N. Patrone*
9:15 Paper 419f: Modeling Adsorption Kinetics of Tetracycline from Aqueous Solution ONTO Natural Bentonite Nanoclay. Elucidating Intraparticle Diffusion Mechanisms — *Uziel Ortiz-Ramos,* ***Roberto Leyva-Ramos***, *Esmeralda Mendoza-Mendoza*
9:30 Paper 419g: Optimal Control of an Ion Exchange Process Under Uncertainty — ***Fred Ghanem***, *Kirti Yenkie*

(420) Division Plenary: Materials Engineering & Sciences Division (Invited Talks)

Wednesday, Nov 10, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 103

Bradley Olsen, Chair
Jodie Lutkenhaus, Co-Chair
Julie Champion, Co-Chair

Sponsored by: Materials Engineering and Sciences Division

8:00 Paper 420a: Precise Materials Synthesis One Layer at a Time — ***Stacey F. Bent***
8:30 Paper 420b: Generic Coarse-Grained Modeling of Ion-Containing Polymers — ***Lisa Hall***
9:00 Paper 420c: Adsorption and Diffusion in Nanoporous Materials: High-Throughput Screening, Machine Learning, and First Principles Simulations— ***Joern Siepmann***
9:30 Paper 420d: Tuning Stickiness on Polyelectrolyte Nanocarriers to Target Cells and Tissues — ***Paula T. Hammond***
10:00 Paper 420e: Dielectric Polymers Under Elevated Temperatures and High Electric Fields — ***Qing Wang***

(421) Emulsions and Foams

Wednesday, Nov 10, 8:00 AM
Sheraton Back Bay, Back Bay Ballroom A

Sepideh Razavi, Chair
Clint Aichele, Co-Chair

Sponsored by: Interfacial Phenomena

8:00 Paper 421a: Growth and Coalescence of Nanoscopic Mesas in Stratifying Micellar Foam Films — ***Chenxian Xu***, *Subinuer Yilixiati, Yiran Zhang, Vivek Sharma*
8:15 Paper 421b: Mechanistic Insights into Lubricant Foaming and Foam Control Using Single Bubble Techniques — ***Vineeth Chandran Suja***, *Suzanne Calhoun, Gerald Fuller*
8:30 Paper 421c: Influences of Surfactant and Salt on Micellar Assemblies and Foam Film Stability — ***Shang Gao***, *Chrystian Ochoa, Vivek Sharma, Samanvaya Srivastava*
8:45 Paper 421e: Characterization of Drop Impact of Oil-in-Water Emulsions on Spinach Leaf — ***Joseph Heng***, *Zhiyun Zhang, Jiakai Lu*
9:00 Paper 421f: Nanoparticle and Surfactant Effects on Oil Drop Migration in Water — ***Xuan Duy Thao Nguyen***, *Tuan Vu, Sepideh Razavi, Dimitrios Papavassiliou*
9:15 Paper 421g: Application of Silane-Treated Silica with Varying Wettability Towards the Demulsification of Surfactant Stabilized Water-in-Oil Emulsions— ***Anirban Ghosh***, *Michael Miranda, Clint Aichele*
9:30 Paper 421h: Magnetically Induced Emulsification and Demulsification of Three-Component Castor Oil/Water/Ethanol Emulsions Stabilized By Cnc@Fe_3O_4 and Lignin@Fe_3O_4 Nanocomposites — ***Mohammad Jahid Hasan***, *Peng Chen, Abhishek Saini, Sarah J. Watzman, Erick S. Vasquez, Esteban E. Urena-Benavides, Fariba Yeganeh*
9:45 Paper 421i: Reversible Emulsification and Demulsification of Oil-in-Oil Emulsions Using Electric Fields — ***Sangchul Roh***, *Nicholas L. Abbott*

(422) Engineering in Aging and Aging-Associated Diseases

Wednesday, Nov 10, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 108

Panagiotis Mistriotis, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

8:00 Paper 422a: *C. Elegans* Lifespan Regulation By Spatiotemporal Activity of DAF-16 — ***Javier Huayta***, *Adriana San Miguel*
8:18 Paper 422b: Exploring the Neurological Exposome for Precision Prevention of Neurodegenerative Diseases — ***Dimosthenis Sarigiannis***, *Ourania Anesti, Nafsika Papaioannou, Antonios Stratidakis, Spyros Karakitsios*
8:36 Paper 422c: Human Ageing at Cell Resolution — ***Jude Phillip***, *Nahuel Zamponi, Debonil Maity, Hasini Jayatilaka, Pei-Hsun Wu, Jeremy Walston, Denis Wirtz*
8:54 Paper 422d: Reprogramming Skeletal Muscle Rejuvenation. — ***Aref Shahini***, *Nika Rajabian, Debanik Choudhury, Shahryar Shahini, Kalyan Vydiam, Joseph Kulczyk, Thy Nguyen, Tyler Santarelli, Izuagie Ikhapoh, Aimee Stablewski, Yali Zhang, Jianmin Wang, Song Liu, Ramkumar Thiyagarajan, Kenneth Seldeen, Bruce Troen, Jennifer Peirick, Pedro Lei, Stelios Andreadis*
9:12 Paper 422e: Development of Human iPSC-Derived Neuron Culture to Study the Contribution of Gene Environmental Interactions to the on-Set of Alzheimer's Disease — ***Junkai Xie***, *Han Zhao, Chongli Yuan, Shichen Wu*
9:30 Paper 422f: Modeling Sympathetic Hyperactivity in Alzheimer's Related Bone Resorption — ***Robert Culibrk***, *Ahmad Arabiyat, Mariah Hahn*
9:48 Paper 422g: High-Content Phenotyping for Analysis of Aging and Its Regulators (Invited Speaker) — ***Adriana San Miguel***

(423) Environmental Advances in Nuclear and Hazardous Waste Processing and Disposal

Friday, Nov 19, 12:30 PM
Virtual, Nuclear Engineering Division (14)

Thong Hang, Chair
Robert Peters, Co-Chair
Philip Schonewill, Co-Chair

Sponsored by: Nuclear Engineering Division

12:30 Paper 423a: Implementation of a New Defoamer in the Defense Waste Processing Facility to Reduce Batch Processing Time and Improve Safety— ***Dan Lambert***, *Wesley H. Woodham, Anthony Howe, Matthew S. Williams, Mason Clark*
12:51 Paper 423b: Water Sorption/Desorption Characteristics in Electrorefiner Salt-Occluded Zeolites — ***Allison Harward***, *Jerry Howard, Claire Decker, Michael Simpson, Krista Carlson, Guy Fredrickson, Tae-Sic Yoo*
1:12 Paper 423c: Performance Assessment for the Low Activity Waste and Intermediate Level Vaults (LAWV and ILV) at the Savannah River Site — *Frank G. Smith III,* ***Maximilian Gorensek***, *L. Larry Hamm*
1:33 Paper 423d: Performance Assessment for Naval Reactor Component Disposal Areas (NRCDA) at the Savannah River Site — ***Thong Hang***, *L. Larry Hamm*
1:54 Paper 423e: Continuous-Flow Centrifugal Solid-Liquid Separation for the Recovery of Rare-Earth Elements Containing Particles from Phosphoric Acid Sludge — ***Gyoung Gug Jang***, *Jong K. Keum, Austin Ladshaw, Patrick Zhang, Costas Tsouris*
2:15 Paper 423f: Effective Adsorption of Chromium from Tannery Wastewater Using Green Synthesis Nano-Zero Valent Iron (GT-nZVI) — *Ahmed S. Mahmoud, M.S. Mahmoud, Ahmed M. Noureldin,* ***Mohamed Mostafa***, ***Robert Peters***
2:36 Paper 423g: Enhanced Biodegradability Assessment of Total Petroleum Hydrocarbon By Implementing a Novel Bioaugmentation Strategy of Indigenous Bacterial Consortium — ***Ipsita D. Behera***, *Asmita Mishra, Ramkrishna Sen, Bhim Charan Meikap*

(424) Fermentation and Process Engineering in Food and Bioprocess Industries

Wednesday, Nov 10, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 107

Ryan Summers, Chair

Shang-Tian Yang, Co-Chair
Jipeng Yan, Co-Chair
Chang Dou, Co-Chair

Sponsored by: Food

8:00: Break
8:18 Paper 424a: Engineering and scale-up of a Conagen production strain for the longevity molecule NMN — ***Jacob E. Vick***
8:36 Paper 424c: The Effects of Flux on the Clearance of Minute Virus of Mice during Constant Flux Virus Filtration — ***Xianghong Qian***, *Rong Fan, Namila Fnu, Dharmesh Kanai, Mi Jin, Ranil Wickramasinghe*
8:54 Paper 424e: High-Throughput Screening of Optimal Process Conditions for ELP Production Via Model Predictive Control — ***Niels Krausch***, *Jong Woo Kim, Sebastian Hans, Sergio Lucia, Peter Neubauer, Mariano Nicolas Cruz Bournazou*
9:12 Paper 113a: A Simple Evaporative Deposition-Thermal Gelation Approach for Facile Fabrication of Biopolymer Films Containing Micropatterned Opal Structures — ***Subhash Kalidindi***, *Hyunmin Yi*
9:30 Paper 113f: Production of Paraxanthine and 7-Methylxanthine from Caffeine Using Genetically Modified *E. coli* — ***Meredith Mock***, *Shelby Mills, Ashley Cyrus, Hailey Campo, Tyler Dreischarf, Sydney Strock, Ryan Summers*
9:48 Paper 424g: [Invited Keynote] Accelerating the Bioeconomy: Leveraging Government Capabilities to Achieve Capital-Light Scale-up and Commercialization — ***Eric Sundstrom***

(425) Fluid Particle Separations in Energy and Environmental Systems

Wednesday, Nov 10, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 301

Seyi Odueyungbo, Chair
Isaac Gamwo, Co-Chair

Sponsored by: Fluid-Particle Separations

8:00: Break
8:20: Break
8:40 Paper 425c: Modeling Barite Precipitation in High Temperature Systems Based on Molecular Statistical Thermodynamics Model — ***Isaac Gamwo***, *Derek Hall, Serguei Lvov, Hseen Baled*

(426) Frontiers in New Materials and Membranes for Bioseparations

Wednesday, Nov 10, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 303

David Latulippe, Chair
Ketki Behere, Co-Chair

Sponsored by: Bio Separations

8:00 Paper 426a: Rethinking Convective Chromatographic Separations — *Riccardo Onesti,* ***Cristiana Boi***
8:20 Paper 426b: Covalent Organic Framework As an Ion Exchange Material for Adsorptive Separation of Biomolecules — ***Imann Mosleh, PhD***, *Ahmad R. Khosropour, Hazim Aljewari, Christina Carbrello, Xianghong Qian, Ranil Wickramasinghe, Alireza Abbaspourrad, Robert Beitle*
8:40 Paper 426c: Scalable Synthesis of Nanoporous Atomically Thin Graphene Membranes for Dialysis and Molecular Separations Via Facile Iso-Propanol-Assisted Hot Lamination — ***Piran Kidambi***
9:00 Paper 426d: Immiscible Liquid-Coated Materials for Bioseparations— ***Justin Hardcastle***, *Daniel P. Regan, Junie Fong, Rushabh Shah, Shao-Hsiang Hung, Aydin Cihanoglu, Jessica Schiffman, Caitlin Howell*
9:20 Paper 426e: Cu-Selective Membrane Adsorbers for Medical Isotope Production — ***Maura Sepesy***, *Benjamin Fugate, Christine Duval*
9:40 Paper 426f: Tuning Structural Defects on Nominal Single-Layered Graphene Oxide Membrane for Selective Separation of Biomolecules — ***Dinesh Behera***, *Bratin Sengupta, Fanglei Zhou, Mirco Sorci, Huazheng Li, Georges Belfort, Miao Yu*
10:00 Paper 426g: The Development of Nanocarbon Immobilized Membrane for Elimination of Thermophilic Bacteria Via Membrane Distillation — ***Indrani Gupta***, *Somenath Mitra*

(427) High-Throughput Techniques in Protein Engineering

Wednesday, Nov 10, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 110

Yongchan Kwon, Chair
Robert Pantazes, Co-Chair

Sponsored by: Bioengineering

8:00 Paper 427a: Engineering a Template-Independent DNA Polymerase for DNA Data Storage and Biosignal Recording Applications — ***Marija Milisavljevic***, *Keith Tyo*
8:18 Paper 427b: Accelerating Protein Engineering Workflows to Synthesize and Screen for New Functional Proteins Containing Non-Canonical Amino Acids— ***Kosuke Seki***, *Yasmine Zubi, Ying Li, Benoit Roux, Jared Lewis, Michael Jewett*
8:36 Paper 427c: Strategies for Quantifying and Enhancing Genetic Code Manipulation in Yeast — *Jessica T. Stieglitz, Kelly Potts, Matthew Zackin, Ming Lei,* ***James Van Deventer***
8:54 Paper 427d: Advancing the Preferential Enrichment of Matrix Metalloproteinase-9 Inhibitors and Their Characterization Using Yeast Display— ***Arlinda Rezhdo***, *Catherine Lessard, James Van Deventer*
9:12 Paper 427e: Detection of Synthetic Peptides As Target Antigens Using Yeast Cell Engineering — ***Monika Arbaciauskaite***, *Yu Lei, Yongku Cho*
9:30 Paper 427f: Deep Mutational Scanning Guided Directed Evolution Reveals Multiple Mechanisms to Improve Enzyme Function — ***Vikas Trivedi***, *Todd C. Chappell, Naveen BK, Anuj Shetty, Gladstone Sigamani, Karishma Mohan, Athreya Ramesh, Pravin R Kumar, Nikhil Nair*
9:48 Paper 427g: Leveraging and Contrasting Multiple Approaches to Engineer Phenylalanine Ammonia-Lyase (PAL) — ***Nikhil Nair***

(428) Industrial Applications in Design and Operations

Wednesday, Nov 10, 8:00 AM
Sheraton Back Bay, Back Bay Ballroom C

Dharik Mallapragada, Co-Chair
Xunyuan Yin, Co-Chair

Sponsored by: Systems and Process Design

8:00 Paper 428a: Nonlinear Predictive Control of an Industrial Selective Catalytic Reduction Unit with Time-Varying Time Delay — ***Elijah Hedrick***, *Katherine Reynolds, Debangsu Bhattacharyya, Stephen E. Zitney, Benjamin P. Omell*
8:21 Paper 428b: Mechanistic Modelling of Reactive Liquid-Liquid Extraction Towers Using Polar PC-SAFT: Industrial Validation and Optimization of Fat/Oil Hydrolysis — ***Pieter Nachtergaele***, *Gürkan Sin, Steven De Meester, Ewout Ruysbergh, Jeroen Lauwaert, Jo Dewulf, Joris Thybaut*
8:42 Paper 428d: A Multi-Agent and Distributed Cloud Computing Approach for Industrial Production Scheduling Model Development and Deployment — ***Adam Kelloway***, *Hojae Lee, Apoorva Sampat, John Wassick*
9:03 Paper 428f: A Surrogate-Based Topological Compartment Model for Counter-Current Spray Dryers. — ***Borja Hernández***, *Mark Pinto, Mariano Martin*
9:24 Paper 428g: Optimal Design and Operation of an Organic Rankine Cycle (ORC) System Driven By Solar Energy with Sensible Thermal Energy Storage— ***Haoshui Yu***, *Truls Gundersen, Gürkan Sin*

(429) Industrial Internet of Things (IIoT), Smart and Soft Sensors in Process Manufacturing and Beyond

Wednesday, Nov 10, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 201

Zhenyu Wang, Chair
Salvador Garcia-Munoz, Co-Chair

Sponsored by: Next-Gen Manufacturing

8:00 Paper 429a: Keynote Talk: Online Measurements for the Petrochemical Industry: Industry 4.0 Trends and Unmet Needs — ***Sherine George***, *James Tate, Paul Cammarata, Eric G. Schmidt, Rod Spitler, John Thibodeaux*
8:35 Paper 429b: Woodchip Moisture Content Estimation Using Short-Range Iot Wi-Fi for the Pulp & Paper Industry — ***Kerul Suthar***, *Jin Wang, Zhihua Jiang, Q. Peter He*
8:58 Paper 429d: Gradient-Weighted Class Activation Mapping (Grad-CAM) Based Explanations for Process Monitoring Results from Deep Neural Networks— ***Abhijit Bhakte***, ***Bairi Sai Vasista***, ***Rajagopalan Srinivasan***
9:21 Paper 429e: A Deep Learning Vision System for Classification of Manufacturing Defects — ***Christopher Hanselman***, *Asit Tiwari, Mamta Venugopal, Lingrui Cai, Yuanfang Guan, Edwin Comparini, Bo Zhang, William R. Prucka*

(431) Large-Scale Models in Systems Biology

Wednesday, Nov 10, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 109

Ashlee Ford Versypt, Co-Chair
Jason E. Shoemaker, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

8:00 Paper 431a: Game Theoretic Approach to Multiple Organ Dysfunction Syndrome — ***Stefanos Papadopoulos***, *Gilles Clermont, Robert Parker*
8:18 Paper 431b: Assessing the Importance of Parametric Uncertainty on Flux Balance Analysis — ***Hoang Dinh***, *Debolina Sarkar, Costas D. Maranas*
8:36 Paper 431h: Epithelial Interferon Production Rates Drive Differential Strain-Specific Immunodynamics — *Emily Ackerman, Jordan Weaver,* ***Jason E. Shoemaker***
8:54 Paper 431d: Patient-Specific CFD Simulations of the Carotid Artery to Predict Stroke — *Leonor N. Teles, Alastair H.S. Lee, Lauren E. Redus, Mauricio Araiza Canizales, Jonathan J. Stone, Priscila Passerotti Vaciski Barbosa,* ***David G. Foster***
9:12 Paper 431e: Recent Enhanced Structural Stress and Tensor Upgrades to Mhawb Tevp Model for Characterization of Human Blood — *Andre Pincot,****Matthew Armstrong***, *Jeffrey S. Horner, Antony Beris*
9:30 Paper 431f: Towards Integrative Mechanistic Models of Mammalian Cell Responses to Extracellular Perturbations: Growth Factors, Hormones, and Cytokines — ***Cemal Erdem***, *Sean M. Gross, Laura M. Heiser, Marc R. Birtwistle*
9:48 Paper 431g: Building an *in silico* Representation of the Tumor Microenvironment One Agent at a Time (Invited Speaker) — ***Neda Bagheri***

(432) Microfluidic and Microscale Flows: Separations and Particulates

Wednesday, Nov 10, 8:00 AM
Sheraton Back Bay, Constitution B

David Leighton, Chair
Hadi Mohammadigoushki, Co-Chair

Sponsored by: Fluid Mechanics

8:00 Paper 432a: Unsteady, Lineal Translation of a Spherical Particle in a Viscoleastic Fluid — ***Mary Joens***, *James Swan*
8:15 Paper 432b: Detection of 3D Position and Orientation of Microparticles Using Holographic Microscopy and Image Moment Techniques — ***Cheng-Wei Tai***, *Adib Ahmadzadegan, Arezoo Ardekani, Vivek Narsimhan*
8:30 Paper 432c: Effect of Particle Softness in Microfluidic Clogging Dynamics— ***Olukayode Majekodunmi***, *Evyatar Shaulsky, Sara Hashmi*
8:45: Break
9:00 Paper 432e: Highthroughput Nanofluidics: A Disposable Virus Enrichment and Purification Ultrafiltration Device for Sensitive and Rapid Screening for Infectious Respiratory Diseases — ***Chenguang Zhang***, *Ceming Wang, Satyajyoti Senapati, Hsueh-Chia Chang*
9:15 Paper 432f: Macrotransport of Chemotactic and Diffusiophoretic Species: Characterizing Species Spreading, Size, and Diffusivity — ***Henry Chu***, *Stephen Garoff, Robert D. Tilton, Aditya S. Khair*
9:30 Paper 432g: Microfluidic Studies of the Production of Polymer Microparticles By Solvent Extraction from Polymer Solution Droplets — *Suryavarshini Sundar, Ghata Nirmal, Calvin Marambo, Ransom Kochhar, Renato A. Chiarella,* ***Arun Ramchandran***
9:45 Paper 432h: Trapping and Assembly of Protocell-like Vesicles in Micro-Scale Pores Via Chaotic Thermal Convection — ***Vijay Ravisankar***, *Yassin A. Hassan, Victor M. Ugaz*
10:00 Paper 432i: Formation of Secondary Dean Vortices in Low-Aspect Ratio Curved Microchannels — ***Minyoung Kim***, *Ali Borhan*
10:15 Paper 432j: Rapid Screening of Active Small Animals Enabled By Open-Surface on-Demand Selection through Digital Mapping — ***Gongchen Sun***, *Hang Lu*

(433) Modeling and Analysis of Chemical Reactors I

Wednesday, Nov 10, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 206

Anthony Dixon, Chair
Gaurav Agrawal, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

8:00 Paper 433a: CH_4 Oxidation over a Pt-Pd/Al_2O_3 Monolith Catalyst: Experiments and Modeling — *Kyle Karinshak, Pak Wing Chen, Austin Morales, Ru-Fen Liu, Lars Grabow,* ***Michael Harold***
8:25: Break
8:50 Paper 433c: Analysis of the Selective Oxidative Dehydrogenation of Ethane over a NiO-SnO_2 Catalyst in an Industrial Packed-Bed Reactor: Heterogeneous Reactor Modelling — ***Carlos Alvarado***, *Jeroen Poissonnier, Carlos Omar Castillo-Araiza,* ***Joris Thybaut***
9:15 Paper 433d: Particle-Resolved CFD Modeling of Packed Bed Reactors: Application to Methane Conversion Processes — ***Laurien Vandewalle***, *Guy B. Marin, Kevin Van Geem*
9:40 Paper 433e: Large-Scale Nonlinear Parameter Estimation with Mixed Effect and Multiresponse Models — ***Thomas Krumpolc***, *Daniel W. Trahan, Daniel Hickman, Lorenz Biegler*
10:05 Paper 433b: Use of Computational Fluid Dynamics to Identify Transport-Derived Errors in Thermal Analysis Testing — ***Rebecca Gibson***, *Mark Simmons, E. Hugh Stitt, Li Liu, Robert Gallen*

(434) Modeling, Control and Optimization of Manufacturing Systems

Wednesday, Nov 10, 8:00 AM
Sheraton Back Bay, Back Bay Ballroom D

Dinesh Krishnamoorthy, Chair
Matthew Ellis, Co-Chair

Sponsored by: Systems and Process Control

8:00 Paper 434a: Multiscale Modeling and Control of Fiber Curl Index to Enhance Fiber Strength in a Pulp Digester — ***Juyeong Jung***, *Hyun-Kyu Choi, Sang Hwan Son, Joseph Kwon, Jay H. Lee*
8:19 Paper 434b: Enabling Real-Time Synergies in Techno-Ecological Systems Using Adaptive Nonlinear Model Predictive Control — ***Utkarsh Shah***, *Joel Paulson, Bhavik Bakshi*
8:38 Paper 434c: Smart Manufacturing and Optimal Operation of an Industrial Air Separation Unit Via Surrogate Modeling and Multiparametric Programming— ***Dustin Kenefake***, *Iosif Pappas, Styliani Avraamidou, Burcu Beykal, Hari S. Ganesh, Yanan Cao, Yajun Wang, Simon Leyland, Jesus Flores-Cerrillo, Efstratios N. Pistikopoulos*
8:57 Paper 434d: Nonlinear Model Predictive Control for Flue Gas Desulfurization — ***Vibhav Dabadghao***, *Lorenz Biegler, Debangsu Bhattacharyya*
9:16 Paper 434e: Integration of Feedback Control and Run-to-Run Control for Plasma Enhanced Atomic Layer Deposition of Hafnium Oxide Thin Films— ***Sungil Yun***, *Yangyao Ding, Yichi Zhang, Panagiotis D. Christofides*
9:35 Paper 434f: Optimal Scheduling of Integrated Processes Under Uncertainty for Biomanufacturing on Mars — ***Soumyajit Sen Gupta***, *Georgios Makrygiorgos, Ali Mesbah, Amor Menezes*
9:54 Paper 434g: Beyond R^2: Cautionary Tales Using Reduced-Order Kinetic Models for Reactor Optimization — ***Kanishka Ghosh***, *Alexander Dowling*
10:13 Paper 434h: Low-Hanging Fruit in High-Purity Distillation Control — ***Mats Friman***

(435) Molecular Simulation and Modeling of Complex Molecules

Wednesday, Nov 10, 8:00 AM
Marriott Copley Place, Salon H/I

Yamil Colón, Chair
Peng Bai, Co-Chair
Kaihang Shi, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

8:00 Paper 435a: Fingerprinting Histone Tail Modifications at Atomistic Resolution in the Human Nucleosome — ***Kathryn Piston***, *Shikha Nangia*
8:15 Paper 435b: Atomistic Simulations of RNA for Characterizing Folding Free Energy Surfaces — ***Gül Zerze***
8:30 Paper 435c: The Dynamic Remodeling of Actin Filament Networks – a Multiscale Approach — ***Sriramvignesh Mani***, *Gregory A. Voth*
8:45 Paper 435d: Distinct Effect of Water on Solvation and Structure of Lipase in Deep Eutectic Solvents Containing Protein Destabilizer and Stabilizers — ***Qi Qiao***, *Jian Shi, Qing Shao*
9:00 Paper 435e: Fast Prediction of Peptide-Surface Interaction without Massive Enhanced Sampling — ***Xin Qi***, *Jim Pfaendtner*
9:15 Paper 435f: Playing Bayesian Jigsaw with PDB Structures: Optimizing Rigid Body Representations for Integrative Modeling of Macromolecular Complexes — ***Tanmoy Sanyal***, *Brian T. Chait, Andrej Sali*
9:30 Paper 435g: Coarse-Grained Molecular Dynamics Study of the Self-Assembly of Triblock Bolaamphiphiles with SAFT-γ Mie CG Forcefield — ***Maziar Fayaz Torshizi***, *Erich A Muller*
9:45 Paper 435h: Novel Model for Electrohydrodynamic Interactions of Polyelectrolytes. — ***Dmitry Kopelevich***, *Jason Butler*
10:00 Paper 435i: Calculating the Entropy of an Entangled Linear Polyethylene Melt Under Shear and Elongational Flows Via Atomistic Simulation — ***Brian Edwards***, *Mohammad Hadi Nafar Sefiddashti, Bamin Khomami*
10:15 Paper 435j: The Development of a Martini Coarse-Grained Model for Rosette Nanotubes — ***Vyshnavi Karra***, *Francisco Hung, Hicham Fenniri*

(436) Next-Gen Manufacturing for Resilience and Sustainability

Wednesday, Nov 10, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 202

Qi Zhang, Chair
Shuyun Li, Co-Chair

Sponsored by: Next-Gen Manufacturing

8:00 Paper 436a: Magnesium Oxychloride Formation Kinetics and Enhanced Water Stability for Sustainable Building Materials Applications — ***Christopher Kitchens***, *Saumye Vashishtha*
8:21: Break
8:42 Paper 436c: Optimization of TEG Dehydration Process in Natural Gas Processing Under Metamodel Uncertainty — ***Rajib Mukherjee***, ***Urmila Diwekar***
9:03 Paper 436d: Mapping Environmental and Economic Analysis of Decentralized Cogeneration Energy Management Centers — ***Nina Monteiro***, *Thomas A. Adams II*
9:24 Paper 436e: Development of an Interactive Software Tool for Designing Industrial Solvent Recovery Processes — ***Jake Stengel***, *John Chea, Emmanuel A Aboagye, Michael Mackley, James Geier, Kirti Yenkie*
9:45 Paper 436f: High Flux CO2 Selective Membranes for Renewable Natural Gas and CO2 Capture — ***Christine Parrish***, *Hannah Murnen, Sudip Majumdar, Ning Shangguan*
10:06 Paper 436g: Optimizing Energy Efficiency of Ammonia Production Via Electrochemical Reaction and Haber-Bosch Process — ***Gbemisola Ojo***, *Kyle Camarda*

(437) Nitrogen Chemistry I: Nitrate Reduction

Wednesday, Nov 10, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 203

Meenesh Singh, Chair
Joseph Gauthier, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

8:00 Paper 437e: Electrochemical Reduction of Nitrates to Ammonia on Oxide Derived Cobalt — ***Nishithan Balaji Chidambara Kani***, *Joseph Gauthier, Aayush Singh, Meenesh Singh*
8:20 Paper 437a: Discovery of Catalysts for the Application of Nitrate Reduction and Water Purification Using Machine Learning Techniques — ***Richard Tran***, *Duo Wang, Ryan Kingsbury, Anubhav Jain, Zachary Ulissi*
8:40 Paper 437b: Controlling Electrocatalytic Nitrate Reduction to Ammonia through Adsorption Energies — *Zixuan Wang, Danielle Richards, Sam Young, Bryan Goldsmith,* ***Nirala Singh***
9:00 Paper 437d: Advanced Reactor Design for Ammonia Production from Electrochemical Nitrogen and Nitrate Reduction — ***Yifu Chen***, *Wenzhen Li*
9:20 Paper 437f: Harnessing Mass Transport to Optimize Ammonia Production during Electrochemical Nitrate Reduction — ***Jinyu Guo***, *Matthew J. Liu, William Tarpeh*
9:40 Paper 437g: Enabling Nitrate Valorization to Ammonia through Electrocatalyst Design — ***Marta Hatzell***, *JeongHoon Lim*

(438) Nucleation and Growth

Wednesday, Nov 10, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 302

Venkateswarlu Bhamidi, Chair
Giovanni Maria Maggioni, Co-Chair

Sponsored by: Crystallization and Evaporation

8:00: Welcoming Remarks
8:03 Paper 438a: Control of Crystal Nucleation By Manipulating the Concentration and Properties of the

Nucleation Precursors — *Wenchuan Ma, Weichun Pan, Michael Sherman,* ***Peter Vekilov***
8:24 Paper 438b: Diffusion Growth Mechanism of Penta-Twinned Ag Nanowires and Cu Nanowires — ***Jianming Cui****, Kristen Fichthorn*
8:45 Paper 438c: Investigating Solute Incorporation into Crystal Kink Sites from Organic Solvents with Molecular Simulation — ***Lakshmanji Verma****, Rajshree Chakrabarti, Jeremy Palmer, Peter Vekilov*
9:06 Paper 438d: Tracking the Emergence of Crystalline Order *Via* Local Structural Analysis — ***Maya Martirossyan****, Julia Dshemuchadse*
9:27 Paper 438e: An Investigation of the Kinetics and Thermodynamics of Nucleation through Composite Cluster Formation from Aqueous Solutions— ***Pelin Su Bulutoglu****, Shiyan Wang, Moussa Boukerche, Nandkishor K. Nere, Doraiswami Ramkrishna*
9:48 Paper 438f: A Simple Accurate Non-Equilibrium Kink Density Model for Centro-Symmetric Molecules — ***Neha Padwal****, Michael F. Doherty*

(439) Particle Agglomeration and Granulation Processes

Wednesday, Nov 10, 8:00 AM
Sheraton Back Bay, Fairfax A/B

Heather Emady, Chair
Brendon Ricart, Co-Chair

Sponsored by: Particle Production and Characterization

8:00 Paper 439a: Binder-Free Twin-Screw Melt Granulation: An Effective Approach to Manufacture High-Dose API Formulations — ***Thamer OMAR****, Ivana Cotabarren, Fernando Muzzio*
8:15 Paper 439c: A Mechanistic Analysis on the Effect of Mixing Dynamics on Granule Microstructure — ***Lalith Venkat Gopal Kotamarthy****, Rohit Ramachandran*
8:30 Paper 439d: Controlled Release of Urea Composites through Formulation and Process Design — ***Camila Garcia Jange****, Carl R. Wassgren, Kingsly Ambrose*

(440) Particulate and Multiphase Flows: Foams and Bubbles

Wednesday, Nov 10, 8:00 AM
Sheraton Back Bay, Constitution A

Amanda Marciel, Chair
Lilian Hsiao, Co-Chair

Sponsored by: Fluid Mechanics

8:00 Paper 440a: Magneto-Capillary Particle Dynamics at Curved Interfaces: Time-Varying Fields and Drop Mixing — *Wenjie Fei, Peter Tzelios,* ***Kyle Bishop***
8:15 Paper 440b: Bubble Rise Behavior in Cornstarch-Water Suspension — *Azin Padash,* ***Boyuan Chen****, Christopher M. Boyce*
8:30: Break
8:45 Paper 440d: Conformal Single Cell Hydrogel Coating with Electrically Induced Tip Streaming of AC Cone — ***Vivek Yadav****, Zehao Pan, Donny Hanjaya-Putra, Hsueh-Chia Chang*
9:00 Paper 440e: Antifoams in Diesel Fuels: Thin Liquid Film Dynamics and Antifoam Mechanisms — ***Suzanne Calhoun****, Vineeth Chandran Suja, Rochelle Kovach, Anil Agiral, Greg Miranda, Gerald Fuller*
9:15 Paper 440f: Predicting the Linear Viscoelasticity of Starch Dispersions during the Initial Stages of Granule Swelling — ***Vivek Narsimhan****, Gnana Prasuna Desam, Jinsha Li, Nadar Laal Dehghani, Ganesan Narsimhan*
9:30 Paper 440g: Performance Benefit of Thermal Coatings for Future in-Space Cryogenic Propellant Transfer Systems — ***Jason Hartwig****, Jacob N. Chung, Samuel Darr*
9:45 Paper 440h: Study the Impact of the Tube Configurations on the Local Heat Transfer Coefficient in Mimicked Fischer Tropsch Bubble Column Reactor— ***Abdulrazaq Alzamily****, Abbas Sultan, Amer Aziz Abdulrahman Abdulrahman, Hayder Al-Naseri, Laith Sabri, Jamal Al-Rubaye*
10:00 Paper 440i: Drainage Via Stratification in Foam Films Made with Polymer-Surfactant Complexes — ***Chenxian Xu****, Chenxian Xu, Vivek Sharma*
10:15 Paper 440j: Rheological Characterization of Dilute Polydisperse Bubble Suspensions — ***Stamatina Mitrou***

(441) Pharmaceutical Discovery, Development, and Manufacturing Forum Awards Ceremony

Wednesday, Nov 10, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 102

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

(442) Practical Applications of Computational Chemistry and Molecular Simulation I

Wednesday, Nov 10, 8:00 AM
Marriott Copley Place, Salon J/K

Martin Sanborn, Chair
Andrea R. Browning, Co-Chair
Jonathan Moore, Co-Chair
Phillip Westmoreland, Co-Chair
Steven G. Arturo, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

8:00 Paper 442a: Simulating the Glass Transition of Steam Cracked Tar— ***Jonathan Saathoff***
8:20 Paper 442b: Multiscale Modeling and Characterization of Radical-Initiated Modification of Molten Polyolefins — ***Weizhong Zou****, Amber Tupper, Nathan Rebello, Duminda Ranasinghe, William Green, Bradley Olsen, Christopher Couch*
8:40: Panel Discussion
9:00 Paper 442d: Thermodynamic Assessment of Low-GWP Refrigerants and Their Performance in Vapor Compression Refrigeration Cycles By Means of Computational Modeling — ***Carlos G. Albà****, Ismail Alkhatib, Fèlix Llovell, Lourdes F. Vega*
9:15: Break
9:30 Paper 442f: Combating COVID-19 Using High Resolution Computational Protein Docking with Natural Drug Products — ***Zirui Wang****, Theodore Belecciu, Daniel Woldring, Michael Bachmann*
9:45: Panel Discussion
10:00 Paper 442h: The Influence of Glycosylation on the Binding of Sars-Cov-2 Spike — *Bradley Harris, Yihan Huang, Shiaki Minami, Karen A. McDonald, Somen Nandi, Priya Shah,* ***Roland Faller***
10:15 Paper 442i: Investigation of Finite-Size Effects of Rutile Titanium Dioxide Clusters — ***Sushree Jagriti Sahoo****, Phanish Suryanarayana, Andrew Medford*

(443) Process Intensification and Modular Manufacturing: Modeling and Simulation

Wednesday, Nov 10, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 209

Ignasi Palou Rivera, Chair
Paul Yelvington, Co-Chair

Sponsored by: Process Intensification & Modular Chemical Processing

8:00 Paper 443a: Modeling Adsorption of Organics-Laden Air from Wood Drying Using the Virtual Moving Bed Model — ***Michael D. Sees****, Kim Tutin, Chau-Chyun Chen*
8:20: Break
8:40 Paper 443c: Process Intensification of Ethylene Oxide Process Using Microfibrous Entrapped Catalyst — ***Chinmoy Basak Mukta****, Selen Cremaschi, Mario Eden, Bruce J. Tatarchuk, Paul Dimick*
9:00 Paper 443d: A Process Intensification Synthesis Approach to Adsorption-Based Reactive Separation Systems — ***Yuhe Tian****, Efstratios N. Pistikopoulos*

(444) Process Intensification in Biorefineries

Wednesday, Nov 10, 8:00 AM
Marriott Copley Place, Exeter

Sridharan Ramaswamy, Chair

Sponsored by: Forest and Plant Bioproducts Division

8:00 Paper 444a: Cross-Flow Separation Characteristics and Piloting of Graphene Oxide Nanofiltration Membrane Sheets and Tubes for Kraft Black Liquor Concentration — ***Chen MA****, Zhongzhen Wang, Scott A. Sinquefield, Meisha L. Shofner, Sankar Nair*
8:15 Paper 444b: Purification of Lignin Monomers from Poplar Derived Reductive Catalytic Fractionation Oils with Counter-Current Chromatography— ***Hoon Choi****, Nathan Soland, Ian McNamara, Stefan Haugen, David Brandner, Eric Tan, Eric M. Karp*
8:30 Paper 444c: SWEET Sorghum Inbreeding to Enhance Sugar Control and Its Perspectives on Ethanol Production — ***Ming-Hsun Cheng****, Anthony J. Studer, Vijay Singh*
8:45 Paper 444d: Visualization and Characterization of Maize (corn stover) Cell Wall Deconstruction By Deacetylation, Ozonation, and Mechanical Refining Pretreatments — *Caroline Frischmon, Bryon Donohoe, Xiaowen Chen,****Sridharan Ramaswamy***
9:00 Paper 444e: Development of a 3D Transport-Reaction MODEL to Understand the Pretreatment Processes in Plant Using RAMAN Spectroscopy— ***Sahana Ramanna****, Bandaru V. Ramarao, Feng Xu, Sridharan Ramaswamy*

(445) Properties and Phase Equilibria for Fuels and Petrochemicals

Wednesday, Nov 10, 8:00 AM
Marriott Copley Place, Fairfield

M R Riazi, Co-Chair
W. Vincent Wilding, Co-Chair

Sponsored by: Fuels and Petrochemicals Division

8:00 Paper 587b: Methane Mass Transfer in Liquid Hydrocarbon Mixtures – Measurement and Modeling in Bulk and in Porous Media — *Zhuofan Shi,****Sheng Hu****, Theodore T. Tsotsis, Kristian Jessen*
8:15 Paper 587a: Screening Inhibitors *in-Situ* to Reduce Asphaltenes Deposition Using Ultra-Small Angle X-Ray Scattering — ***Rizwanur Rahman****, Weiyi Kong, Katie Izatt, Cesar Ovalles, Estrella Rogel, Michael P. Hoepfner*
8:30 Paper 356n: A Liquid Heat Capacity Limit for Organic Compounds— ***Joseph Bloxham****, Paul Mathias*

(446) Reaction Engineering in Pharmaceuticals and Fine Chemicals

Wednesday, Nov 10, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 207

Gaurav Giri, Chair
Onkar Manjrekar, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

8:00 Paper 446a: Continuous Ligand-Free Suzuki-Miyaura Cross-Coupling Reactions in a Packed Bed Flow Reactor Using an Easily Synthesized Siloxane Network-Supported Palladium Catalyst — ***Bradley Davis****, Jeffrey A. Bennett, Milad Abolhasani*
8:18 Paper 446b: Engineering Composite Hollow Fiber As a Heterogeneous Catalyst and Continuous-Flow Microfluidic Reactor for Sustainable Production of Fine Chemicals — ***Ali Rownaghi***
8:36 Paper 446c: Development and Validation of Enzymatic Kinetic Model for the Synthesis of Cephalexin and Amoxicillin By Penicillin G Acylase at High Substrate and Product Concentrations — ***Patrick Harris****, Ronald Rousseau, Martha Grover, Andreas Bommarius*
8:54 Paper 446e: Optimizing Multistep Continuous Flow Organic Synthesis with Bayesian Optimization and Robotics — ***Anirudh M.K. Nambiar****, Christopher P.*

Breen, Travis Hart, Tim Kulesza, Timothy Jamison, Klavs Jensen
9:12 Paper 446f: A Process Monitoring Approach for Multistep Continuous Flow Pharmaceutical Manufacturing: Combining Dynamic Modeling and IR Spectroscopy with Changepoint Analysis — ***Cameron Armstrong***, *Yuma Miyai, Anna Formosa, Pratiik Kaushik, Luke Rogers, Thomas Roper*
9:30 Paper 446g: Heat Transfer Characterization in Flow Reactors for Continuous Pharmaceutical Oxidations — ***Fatou Baka Diop***, *Gabriela Chong, Emily Gonzales, Andrew R Teixeira*
9:48 Paper 446h: Identification of Reaction Pathways Using in-Line Process Analytical Technology (PAT): UV-Vis Spectroscopic Approach — ***Farshid Mohammadparast***, *Ravi Teja Addanki Tirumala, Sundaram Bhardwaj Ramakrishnan, Marimuthu Andiappan*

(447) Recycling and Upcycling of Plastic Waste

Wednesday, Nov 10, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 200

Wan-Ting Chen, Chair
Jeffrey Seay, Co-Chair
Shelby Browning, Co-Chair

Sponsored by: Waste Plastics

8:00: Break
8:25: Break
8:50 Paper 447c: Computational Prediction of Polymer Solubilities and Its Application in Multilayer Plastic Film Recycling — ***Panzheng Zhou***, *Kevin Sanchez-Rivera, George Huber, Reid Van Lehn*
9:15 Paper 447d: Calibration of a CFD-DEM Fluidised Bed Simulation for Plastic Recycling Using Positron Emission Particle Tracking — ***Dominik Werner***
9:40 Paper 447e: Use of Waste Plastic in Asphalt Binder: Theoretically and Experimentally Justified Identification of Compatible Blends — ***Andrew Peters***, *Aniruddha Chowdhury, S.M. Rahat Rahman, Anwar Shafe, Roksana Hossain, Nazimuddin Wasiuddin*

(448) Sustainable Engineering Forum Plenary (Invited Talks)

Wednesday, Nov 10, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 312

Fengqi You, Chair
Mark Mba Wright, Co-Chair

Sponsored by: Sustainable Engineering Forum

8:00 Paper 448a: Reinventing the Chemical/Materials Company: Transitioning to a Sustainable Circular Enterprise — ***George Stephanopoulos***, *Bhavik Bakshi, George Basile*
8:45 Paper 448b: A Multi-scale Systems Engineering approachtowards Sustainable Energy Transition Strategies — ***Efstratios N. Pistikopoulos***
9:30 Paper 650g: System-Level Approaches for Intensifying the CO_2Electrolysis Process — ***Saket Sanjay Bhargava***, *Daniel Azmoodeh, Prithviraj Chumble, Sujay Someshwar, Paul Kenis*
9:50 Paper 448c: Sustainable synthesis of NH_3 via electrochemical reduction of N_2 on an earth abundant Cu gas diffusion electrode at ambient conditions— ***Nishithan Balaji Chidambara Kani***
10:10 Paper 448d: Increasing energy yield from dusty solar panels by a new generation of electrostatic based self-cleaning technology — ***Alexander Orlov***

(449) Teaching Data Science to Students and Teachers I

Wednesday, Nov 10, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 306

Martha Grover, Chair
Phillip Westmoreland, Co-Chair

Sponsored by: Bridging the Skills Gap in Chemical Engineering

8:00 Paper 449a: Teaching Process Data Analytics and Machine Learning— ***Richard D. Braatz***, *Weike Sun, Brian W. Anthony*
8:30 Paper 449c: Teaching Big Data Science to Undergraduate Students in the University of Iowa — ***Jun Wang***, *Joseph S. Gomes, Charles Stanier*
9:00 Paper 449d: Textile: Tutorials in Experimentalist Interactive Learning— ***Hawley Helmbrecht***, *Elizabeth Nance*
9:30 Paper 449e: Teaching Artificial Intelligence to Chemical Engineers: Experiences from a 35-Year-Old Course — ***Venkat Venkatasubramanian***
10:00: Panel Discussion

(450) Thermal Energy Storage

Wednesday, Nov 10, 8:00 AM
Sheraton Back Bay, Back Bay Ballroom B

Gus Georgeton, Chair

Sponsored by: Transport and Energy Processes

8:00 Paper 450c: Redox Thermodynamics of Fe-Doped Magnesium Manganate for Thermochemical Energy Storage — ***Jayni Hashimoto***, *Alicia Bayon, Christopher L. Muhich*

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

Wednesday, Nov 10, 8:00 AM
Marriott Copley Place, Salon C/D

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

Sponsored by: Thermodynamics and Transport Properties

8:00 Paper 451a: Individual and Mean Ionic Activity Coefficients: Insight from Molecular Dynamics Simulations — ***Sina Hassanjani Saravi***, *Athanassios Panagiotopoulos*
8:16 Paper 451b: Designing Molten Salt Eutectics: A Combined Thermodynamic Modeling and Machine Learning Approach — ***Ashwin Ravichandran***, *Shreyas Honrao, Eric Fonseca, John W. Lawson*
8:32 Paper 451c: Tuning Deep Eutectic Solvent Properties with Phenolic-Derivative Hydrogen Bond Donors — ***Derrick Poe***, *Xiaoyu Wang, Yong Zhang, William Dean, Jeffrey Klein, Burcu Gurkan, Edward J. Maginn*
8:48: Break
9:04 Paper 451e: Multi-Scale Modeling of Amine-Based Water-Free Solvents for CO_2 Capture — ***Ismail Alkhatib***, *Daniel Bahamon, Omar Khalifa, Lourdes F. Vega*
9:20 Paper 451f: A Theory of Localized Excitations in Supercooled Liquids— ***Muhammad Hasyim***, *Kranthi K. Mandadapu*
9:36 Paper 451g: Vapor-Liquid Equilibria of Binary and Ternary Mixtures Containing Ethyl Lactate As Entrainer for the Separation of Binary Azeotropic Mixture Ethyl Acetate + Ethanol — ***Hiroyuki Matsuda***, *Takaki Onoo, Jun Koyama, Hibiki Tanaka, Kiyofumi Kurihara, Katsumi Tochigi*
9:52 Paper 451h: Predicting the Temperature Dependence of Sucrose and α-Glycine Aqueous Solubility from Thermodynamic Data Measured at a Single Temperature — ***Andrew Manson***, *Andrew Coll, Leo Lue, Jan Sefcik*
10:08 Paper 451i: Vapor-Liquid-Liquid Phase Transition of a Chiral Tetramer Model — ***Yiming Wang***, *Frank H. Stillinger, Pablo Debenedetti*

(453) Young Faculty Forum (Invited Talks)

Wednesday, Nov 10, 8:00 AM
Sheraton Back Bay, Republic Ballroom A

Christine Duval, Chair
Elif E. Miskioglu, Co-Chair
Maura Sepesy, Co-Chair

Sponsored by: Young Faculty Forum

8:00 Paper 453a: Focus on What Matters – Advice on How to Spend More Time Doing the Things You Enjoy and Manage Your Academic Life — ***Jim Pfaendtner***
8:30 Paper 453b: Talk from Margo Vigeant — ***Margot Vigeant***

(454) John M. Prausnitz AIChE Institute Lecture

Wednesday, Nov 10, 11:15 AM
John B. Hynes Veterans Memorial Convention Center, Ballroom B

Richard Braatz, Chair

Sponsored by: Awards Committee

11:15 Paper 454a: Viruses, Immunity, and Vaccines — ***Arup K. Chakraborty***

(456) Adsorbent Materials: MOFs

Wednesday, Nov 10, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 305

Youssef Belmabkhout, Chair
Stephen DeWitt, Co-Chair

Sponsored by: Adsorption and Ion Exchange

12:30: Break
12:49 Paper 366e: Effect of Water Loading on the Stability of Dmof-1— ***Carmen Chen***, *Zhenzi Yu, David Sholl, Krista Walton*
1:08 Paper 456d: Controlled Demolition and Reconstruction of Metal-Organic Frameworks By Acid Gas Treatment and Linker Insertion — ***Arvind Ganesan***, *Stephen Purdy, Katharine L. Page, David Sholl, Sankar Nair*
1:27 Paper 456h: A Systematic Study of MOFs Containing Different N-Sites for Hydrogen Sulfide Adsorption — ***Chengzhai Wang***, *Krista Walton*
1:46: Break
2:00 Paper 456f: Simultaneous Interlayer and Intralayer Space Control in Two-Dimensional Metal−Organic Frameworks for Alkyne/Alkene Separation — *Jin Shen, Xin He, Tian Ke, Rajamani Krishna, Jasper M. Van Baten, Zongbi Bao, Mircea Dincă, Zhiguo Zhang,* ***Yang Qiwei***, *Ren Qilong*
2:19 Paper 456i: Design of Porous Material Based Electronic Nose for Gas Sensing: Impact of Adsorbent Equilibrium and Kinetics — ***Ashwin Kumar Rajagopalan***, *Camille Petit*
2:38 Paper 456b: Understanding Carbon Monoxide Binding and Interactions in M-MOF-74 (M = Mg, Mn, Ni, Zn) — ***Ishan Pandey***, *Chi-Ta Yang, Li-Chiang Lin, Chau-Chyun Chen, Joshua Howe*

(457) Advanced Electrochemical Energy Storage Technologies I

Wednesday, Nov 10, 12:30 PM
Sheraton Back Bay, Back Bay Ballroom B

Gang Wu, Chair
Ling Fei, Co-Chair

Sponsored by: Transport and Energy Processes

12:30 Paper 457a: Electrochemical Intercalation of Protons into Fluorine-Doped Molybdenum Oxide: A Positive Electrode for Rechargeable Aqueous Aluminum Metal Batteries — *Ankur L. Jadhav, Leo Gordon, MChem, MPhil,* ***Robert Messinger***
12:55: Break
1:20 Paper 457c: Design and Characterization of a Neutron-Friendly Lithium-Ion Battery Coin Cell for Extreme Fast-Charging — ***Maha Yusuf***, *Jacob LaManna, Molleigh Preefer, Partha Paul, David Agyeman-Budu, Michael Toney, Johanna Weker*

1:45 Paper 457d: In Operando Study of All-Solid-State Lithium Batteries Coupling Thioantimonate Superionic Conductors with Metal Sulfide — ***Xiao Sun**, Alyssa Stavola, Daxian Cao, Andrea Bruck, Joshua Gallaway, Hongli Zhu*

(458) Advanced Separations Processes in Bioprocessing and Biomaterials

Wednesday, Nov 10, 12:30 PM
Marriott Copley Place, Provincetown

Bandaru V. Ramarao, Chair
Sridharan Ramaswamy, Co-Chair

Sponsored by: Forest and Plant Bioproducts Division

12:30: Break
12:45 Paper 458b: Thiol-functionalized Hyper-Cross-Linked Milk Protein polymers for Mercury Removal — ***Maryam Davaritouchaee**, Ahmadreza Khosropour, Alireza Abbaspourrad*
1:00 Paper 458c: Effect of Selective Impurities on Carbon Capture from Biogas Using Deep Eutectic Solvents — ***Thomas Quaid**, Toufiq Reza*
1:15 Paper 458d: Dewatering/Dehydration of Ethanol Using Ultrasound
1:30 Paper 458e: Design, Simulation, and Validation of 3-D Printed Hydrocyclones for Microbial Cell Concentration — *Aiden Truettner, Elizabeth Hoekstra, Jacob Franz, Ravneet Kaur Kailey, Joshua Pearce, **Rebecca Ong***
1:45 Paper 458f: Switching Bioprocesses into Zero-Waste Virtual Power Plants By Flexible Operation of Electrochemical pH-Swing Extraction Processes— ***Marcel Gausmann**, Andreas Jupke*
2:00 Paper 458g: Electrokinetic Modeling of Salt Transport and Rejection in Graphene Oxide Nanofiltration Membranes — ***Zhongzhen Wang**, Qiang Fu, Chunyan Xu, Chen MA, Scott A. Sinquefield, Meisha L. Shofner, **Sankar Nair***

(459) Advances in Clean Energy R&D (Invited Talks)

Tuesday, Nov 16, 12:30 PM
Virtual, Sustainable Engineering Forum (23)

Madhava Syamlal, Chair
Chunshan Song, Co-Chair

Sponsored by: Sustainable Energy

12:30 Paper 459a: The Role of Carbon Capture in Meeting Net-Zero Carbon Goals — ***Jennifer Wilcox***
1:00 Paper 459b: Clean Energy and Decarbonization Research, Development and Demonstration at Oak Ridge National Laboratory — ***Xin Sun***
1:30 Paper 459c: Getting to Zero Emissions: The Need for Nuclear Energy— ***Ripudaman Malhotra***
2:00 Paper 459d: High-Temperature Co-Electrolysis of CO_2 and H_2O on Lanthanum Ferrite-Type Perovskite Oxide Cathodes — *Dhruba Jyoti Deka, Seval Gunduz, Jaesung Kim, Matt Ferree, Taylor Fitzgerald, Yingjie Shi, Jean-Marc Millet, Jeffrey T. Miller, Anne Co, **Umit S. Ozkan***

(460) Advances in Process Design II

Wednesday, Nov 10, 12:30 PM
Sheraton Back Bay, Back Bay Ballroom C

Gonzalo Guillén-Gosálbez, Co-Chair
M M Faruque Hasan, Co-Chair
Salih Emre Demirel, Co-Chair

Sponsored by: Systems and Process Design

12:30 Paper 460a: Multi-Objective Optimization for the Synthesis of Reliable and Inherently Safer Process Plants — ***Andrea Ortiz Espinoza**, Yixin Ye, Arturo Jiménez-Gutiérrez, Ignacio Grossmann*
12:51 Paper 460b: Optimization Opportunities for Stand-Alone Liquid Air Energy Storage — *Zhongxuan Liu, **Truls Gundersen***
1:12 Paper 460c: A Spatial Superstructure Approach to the Optimal Design of Modular Processes and Supply Chains — ***Yue Shao**, Victor M. Zavala*
1:33 Paper 460d: Design Space Identification Via Multi-Parametric Programming — ***Steven Sachio**, Cleo Kontoravdi, Maria Papathanasiou*
1:54 Paper 460e: Using Representative Days for the Design of Renewable-Based Utility Plants — *Salvador Pérez Uresti, Ricardo Pinto de Lima, **Mariano Martin**, Arturo Jiménez-Gutiérrez*
2:15 Paper 460f: Integrated Multiscenario Sensor Network Design for Data Reconciliation and Process Optimization — ***Jiawen Wei**, Qi Zhang, Zhihong Yuan*
2:36 Paper 460g: Generalized Superstructure-Based Distillation Network Synthesis — ***Joonjae Ryu**, Christos Maravelias*

(461) Advances in Zeolite Science and Technology III - New Horizons (Invited Talks)

Wednesday, Nov 10, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 208

Kathryn Bjorkman, Chair
Thomas Degnan, Co-Chair

Sponsored by: Advances in Zeolite Science and Technology

12:30 Paper 461a: Influence of Clusters of Brønsted Acid Sites on Methanol Dehydration Rates in Zeolite Catalysts — ***David Hibbitts***
12:55 Paper 461b: Leveraging High Throughput Simulations for the Synthesis of Small Pore Zeolites with Repurposed Osdas — ***Yuriy Roman**, Daniel Schwalbe-Koda, Soonhyoung Kwon, Cecilia Paris, Estefania Bello-Jurado, Zach Jensen, Elsa Olivetti, Tom Willhammar, Avelino Corma, Manuel Moliner, Rafael Gomez-Bombarelli*
1:20 Paper 461c: *A Priori* Control of Zeolite Phase Competition with High-Throughput Simulations — ***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*
1:45 Paper 461d: Guiding the Synthesis Routes to Prepare Small Pore Zeolites for Environmental and Industrial Applications — *Estefania Bello-Jurado, Cecilia Paris, Daniel Schwalbe-Koda, Soonhyoung Kwon, Tom Willhammar, Avelino Corma, Yuriy Roman, Rafael Gomez-Bombarelli, **Manuel Moliner***
2:15 Paper 289b: Mechanisms and Rates of Catalyst Deactivation in Methanol-to-Hydrocarbons Conversion — ***Aditya Bhan***

(462) Applications of Therapeutic and Enzymatic Protein Engineering

Wednesday, Nov 10, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 110

Lawrence Stern, Chair
Jamie Spangler, Co-Chair

Sponsored by: Bioengineering

12:30 Paper 462a: Engineered Immunocytokines Improve Delivery of IL-2 to Pro-Inflammatory Cells and Promote Anti-Tumor Activity — ***Elissa Leonard**, Jamie Spangler*
12:48 Paper 462b: Directed Evolution of TIMP-Based Protein Scaffolds for Metalloproteinase Inhibition — ***Maryam Raeeszadeh Sarmazdeh**, Linh Do, Mari Toumaian, Alexander Bolt, Imam Sanousi*
1:06 Paper 462c: NAD(H)-Peg Swing Arms Improve Both the Activities and Stabilities of Modularly-Assembled Transhydrogenases Designed with Predictable Selectivities — ***Nadim Massad**, Scott Banta*
1:24 Paper 462d: Single c-to-t Substitution Using Engineered apobec3g-ncas9 Base Editors with Minimum Genome- and Transcriptome-Wide Off-Target Effects — ***Xue Sherry Gao***
1:42 Paper 462f: Antibody-Lectin Bispecifics for Targeting Glyco-Immune Checkpoints — ***Jessica C. Stark**, Melissa Gray, Simon Wisnovsky, Carolyn Bertozzi*
2:00 Paper 462g: Engineering Ribosomal Natural Products As New Antimicrobials — ***Aaron Link***

(463) Applied Formulation Design

Wednesday, Nov 10, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 102

Blair Brettmann, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

12:30 Paper 463a: Advanced Formulation of Co-Processed Ionic Liquid Drugs *Via* Spray Drying for Incorporation into Solid Dosage Forms — ***Michael Stocker**, Evangelia Tsolaki, Anne Marie Healy, Steven Ferguson*
12:54 Paper 463d: Rapid Manufacturing Route Conversion Based on the Role of Shear and the Effect of Shear on the Formulation — ***Fernando Muzzio**, James Scicolone, Jingzhe Li*
1:18 Paper 463e: An *in silico* Tool for Quantitative Kinetic Predictions of API Degradation — ***Haoyang Wu**, Alon Grinberg Dana, Duminda Ranasinghe, William Green, Jason Mustakis, Gregory Sluggett, Todd Zelesky, Frank Pickard IV, Geoffrey Wood*
1:42 Paper 463f: Structure - Function Analysis of Lipids for the Development of Advanced Excipients for Pharmaceutical Manufacturing — ***Sharareh Salar-Behzadi**, Carolina Corzo, Eleonore Fröhlich, Andreas Zimmer, Ioannis Koutsamanis, Martin Spoerk, Carolina Alva, Moaaz Abdelhamid, MSc, Ana Belén Ocampo, Dirk Lochmann, Sebastian Reyer, Tanja Freichel*
2:06 Paper 103c: Implementation of a Methodology for Selection of an Appropriate Tracer to Measure the Residence Time Distribution (RTD) of Continuous Powder Blending Operations — ***Sonia M. Razavi**, Andres Roman-Ospino, Atul Dubey, Marianthi Ierapetritou, Fernando Muzzio*
2:30 Paper 103f: Development of Discrete Element Method Calibration Approach for Pharmaceutical Applications — ***Pooja Bhalode**, Yi Tao, Fernando Muzzio, Marianthi Ierapetritou*

(464) Assessing and Evaluating Student Learning and Performance

Wednesday, Nov 10, 12:30 PM
Sheraton Back Bay, Liberty B/C

Matthew Cooper, Chair
Jennifer Cole, Co-Chair
Monica Lamm, Co-Chair

Sponsored by: Education

12:30 Paper 464a: Putting the Focus on Learning and Skill Development through Mastery Grading in Thermodynamics — ***Adam Ekenseair***
12:48 Paper 464b: Beyond Right and Wrong: Performance and Persistence in Solving Scaffolded, Randomized, and Auto-Graded Homework Problems — *Kayla Chapman, **Matthew Liberatore***
1:06 Paper 464d: Data-Driven Continuous Improvement Strategies for Asynchronous Online Courses — ***Justin Vento**, Matthew Cooper*
1:24 Paper 464f: Effort-Based Grading of Homework — ***Carl Lund***
1:42 Paper 464g: Authentic Assessment in Chemical Engineering Using Virtual Laboratories — ***Milo Koretsky***

(465) Biodegradable Polymers from Forest Resources - Sustainable Biomaterials

Wednesday, Nov 10, 12:30 PM
Marriott Copley Place, Exeter

Bandaru V. Ramarao, Chair
Deepak Kumar, Co-Chair

Sponsored by: Forest and Plant Bioproducts Division

12:30 Paper 465a: Process Design and Scale-up Study for the Production of Polyol-Based Biopolymers from

Sawdust — *Jose Enrique Roldán-San Antonio,**Edgar Martin Hernandez**, Rodrigo Briones, **Mariano Martin***
12:45 Paper 465b: Phasins Employed By *Rhodopseudomonas Palustris*CGA009 for Bioplastic Production from Lignocellulosic Biomass — ***Brandi Brown**, Dianna Long, Cheryl Immethun, Mark Wilkins, Rajib Saha*
1:00 Paper 465c: Engineering Functional Materials from Cellulose Nanocrystals By Exploring Their Structure and Property Relationships — ***Ananya Ghosh**, ZhongYang Cheng, Zhihua Jiang*
1:15 Paper 465d: Discovery and Development of New Sustainable Polyesters from Biomass — ***Wontae Joo**, Sarah Av-Ron, K'yal Bannister, Omar Tantawi, Desiree Plata, Kristala Prather, Bradley Olsen*

(466) Biomaterials in Industry and the Clinic

Monday, Nov 15, 8:00 AM
Virtual, Materials Engineering and Sciences Division (08)

Latrisha K. Petersen, Chair
Eun Ji Chung, Co-Chair
Forrest Kievit, Co-Chair

Sponsored by: Biomaterials

8:00 Paper 466a: From Academic Research to Industrial Product: Avoiding the Translational Blues — ***Guillermo Ameer***
8:30 Paper 466c: *Suture Technology – a Partial Review of the Most Ubiquitous Wound Closure Modality* — ***Davide Miksa**, Daniel Steiger*
9:00 Paper 466b: Perfluoropolyether (PFPE) Modified Polyurethane Material with Antifouling Surface Properties for Catheter Devices — ***He Bai***
9:30 Paper 466d: Smart Antibacterial and Antifungal Biomaterials — ***Anita Shukla***
10:00 Paper 466e: Design Strategy and Applications of Citrate-Based Photoluminescent Materials — ***Jian Yang***

(467) Bionanotechnology Graduate Student Award Session I

Wednesday, Nov 10, 12:30 PM
Marriott Copley Place, Simmons

Catherine Fromen, Chair
Lorraine Leon, Co-Chair
Elizabeth Nance, Co-Chair

Sponsored by: Bionanotechnology

12:30 Paper 467a: Gold Nanoparticle-Enhanced siRNA Silencing in Plants Can Occur Independent of NP Internalization — ***Natalie Goh**, Huan Zhang, Jeffrey Wang, Salwan Butrus, Gozde Sultan Demirer, So-Jung Park, Markita Landry*
12:50 Paper 467b: Developing Thin, Drug-Eluting Topical Ocular Gels Formed By Administration of Low Concentration, Thermoreversible Polymer Solutions in Hypotonic Aqueous Vehicles — ***Tung Heng Hsueh**, Yoo Chun Kim, Matthew Shin, Sean Hackett, Justin Hanes, Laura Ensign*
1:10 Paper 467c: Award Submission: Development of Stable Targeted Nano-, Encapsulated Manganese Oxide (NEMO) Particles for Early Breast Cancer Diagnosis By MRI — ***Celia Martinez de la Torre**, Kasey Freshwater, Margaret Bennewitz*
1:30 Paper 467d: Graduate Student Award Session: Liposome and Polyelectrolyte Layers Derived Single Shot Vaccine Platform for Controlled Release of Inactivated Chikungunya Virus — ***Rashi Porwal**, Anuj Sharma, Srivatsan Kidambi*
1:50 Paper 467e: Liposomal Drug Delivery for Wound Infections in Diabetic Foot Ulcers — ***Pranali Buch**, Edgar D. Goluch*
2:10 Paper 467f: Near-Infrared Catecholamine Nanosensors Reveal Disruptions in Dopamine Release in Huntington's Disease Mouse Models — ***Sarah Yang**, David Schaffer, Markita Landry*

(468) Catalyst Design, Synthesis, and Characterization II - Atomically Dispersed Catalysts

Wednesday, Nov 10, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 205

Nathaniel Eagan, Chair
Madelyn R. Ball, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

12:30 Paper 468a: Postsynthetic Routes to Atomically Dispersed M–N–C Catalysts Inspired By Surface Organometallic Chemistry — ***Jason S. Bates**, Qiang Gao, Abdulhadi Al-Omari, Thatcher W. Root, Shannon S. Stahl*
12:50 Paper 468b: Theoretical Insights into the Heterogeneous Hydroformylation of Ethylene on Atomically Dispersed Rh-Oxide Promoter Pairs on γ-Al_2O_3 Support — ***Seungyeon (Lina) Lee**, Ji Qi, Insoo Ro, Phillip Christopher, Stavros Caratzoulas, Dionisios Vlachos*
1:10 Paper 468c: Creation of Single Pt Atoms in Znox Nests in Dealuminated Zeolite Beta for Propane Dehydrogenation — ***Liang Qi**, Alexis T. Bell*
1:30 Paper 468d: Dilute Alloys of Palladium in Indium Supported on γ-Al_2O_3 for the Selective Hydrogenation of CO_2 to Methanol — ***Abdulaziz Alamer**, Mengyao Ouyang, Faisal Alshafei, Jeffrey T. Miller, Maria Flytzani-Stephanopoulos, E Charles Sykes, Vasilios Manousiouthakis, Nathaniel Eagan*
1:50 Paper 468e: Method to Produce High Densities of Isolated Atoms Regardless of the Support Functional Groups — ***Abolfazl Shakouri**, Horie Adabi Firouzjaie, Stavros Karakalos, William Mustain, Christopher Williams, John R. Regalbuto*
2:10 Paper 468g: Dynamic Coordination of Dilute Alloys Under Reactive Environments: Supported Ag-Pt Nanoparticle Catalysts — ***Jordan Finzel**, Phillip Christopher*
2:30 Paper 468f: Using Reductive Approach to Synthesize Atomically Dispersed Pt Catalysts Via Strong Metal Support Interaction — ***Sufeng Cao**, Zhichun Si, Maria Flytzani-Stephanopoulos, Dunwei Wang, E Charles Sykes*

(469) Charged and Ion Containing Polymers 1

Wednesday, Nov 10, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 105

Samanvaya Srivastava, Chair
Xiaoxue Wang, Co-Chair
Whitney Loo, Co-Chair
Hee Jeung Oh, Co-Chair

Sponsored by: Polymers

12:30 Paper 469a: Impact of Surface-Induced Order on Ion Conductivity in Block Copolymer Electrolytes — ***Jonathan Coote**, Gila E. Stein, Joshua Sangoro*
12:45 Paper 469c: Superionicity in Structurally Inhomogeneous, Solvent-Free Polymeric Zwitterionic Liquids Doped with Lithium Salts — ***Seamus Jones**, Howie Nguyen, Peter Richardson, Yan-Qiao Chen, Kira Wyckoff, Craig J. Hawker, Raphaële Clément, Glenn H. Fredrickson, Rachel Segalman*
1:00 Paper 469d: Polymer Electrolytes in Heterogenous Media — ***Monica Olvera De La Cruz**, Trung Nguyen, Felipe Jimenez-Angeles*
1:30 Paper 469e: Role of Solvation Site Segmental Dynamics on Ion Transport in Ethylene-Oxide Based Polymer Electrolytes — ***Peter Bennington**, Chuting Deng, Daniel Sharon, Michael Webb, Juan J. de Pablo, Paul F. Nealey, Shrayesh Patel*
1:45 Paper 469g: Side-Chain Engineering of Mixed Conducting Polymers Using Coarse-Grained Molecular Dynamics — ***Aditi Khot**, Brett Savoie*
2:00 Paper 469h: Effect of Interfacial Polymer Layer on Ion Transport in Hybrid Ceramic-Polymer Solid Electrolytes — ***Manuela Ferreira**, Y. Elaine Zhu*
2:15 Paper 469i: Silicone Based Ionoelastomers for Soft, Electroactive Devices— ***Matthew McBride**, Hyeongjun Kim, Owen Lee, Ryan Hayward*
2:30 Paper 523f: Dynamic Regimes in Entangled Asymmetric Coacervates with Added Salt — ***Christian Aponte-Rivera**, Michael Rubinstein*

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

Wednesday, Nov 10, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 300

Geoffrey Geise, Co-Chair
Hee Jeung Oh, Co-Chair

Sponsored by: Membrane-Based Separations

12:30 Paper 470a: Counter-Ion Transport in Highly Charged and Low Water Content Ion-Exchange Membranes — ***Jovan Kamcev***
12:45 Paper 470c: Facilitated Transport Mechanisms of Ion-Selective Membranes with Fixed Coordination Sites — ***Ryan M. DuChanois**, Menachem Elimelech*
1:00 Paper 470d: Ultrathin Perfluorinated Sulfonic Acid Ionomer Membranes for Vanadium Redox Flow Battery: The Effect of Ordered Nanomorphology and Annealing on Ion-Transport Properties — ***Jongmin Kim**, Soonyong So, Hee-Tak Kim, Siyoung Choi*
1:15 Paper 470e: Impact of Sulfonation Degree and Nanoparticle Surface Chemistry on Ion Selectivity in Sulfonated Ionomer Nanocomposites — ***Xueting Wang**, Mayura Silva, Stephen Creager, Eric M. Davis*
1:30 Paper 470f: Sulfonated Oligo-Sulfone Ionomer: Proton Transport-Property Under Thin Film Confinement and Structural Characterization Thereof.— ***Shyambo Chatterjee**, Rajesh Keloth, Shudipto K. Dishari*
1:45 Paper 470g: Assembly of Nanoparticle-Polyelectrolyte Membranes at Water-Water Interfaces — ***Wilfredo Mendez**, Kathleen J. Stebe, Daeyeon Lee*

(471) Computational Studies of Self-Assembly

Wednesday, Nov 10, 12:30 PM
Marriott Copley Place, Salon H/I

Julia Dshemuchadse, Chair
Sumit Sharma, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

12:30 Paper 471a: Generalizing Strong-Segregation Theory to Arbitrarily Complex Block Copolymer Geometries — ***Michael Dimitriyev**, Abhiram Reddy, Gregory M. Grason*
12:45 Paper 471b: Universal Phase Behavior of Linear, Comb, and Bottlebrush Diblock Copolymers Via Self Consistent Field Theory — ***Daniel Vigil**, Timothy Quah, Dan Sun, Kris Delaney, Glenn H. Fredrickson*
1:00 Paper 471c: Structure and Stability of Self-Assembled Aqueous AOT Aggregates in Molecular Dynamics Simulations — ***Vance Jaeger**, Anuradha Bhat, Michael Harris*
1:15 Paper 471d: Controlling the Association of Pfas Surfactants in Aqueous Environments — *Samhitha Kancharla, Dengpan Dong, Dmitry Bedrov, Marina Tsianou, **Paschalis Alexandridis***
1:30 Paper 471e: Using Stoichiometry to Enhance Binary Colloidal Assembly— ***Ronald LaCour II**, Timothy C. Moore, Sharon Glotzer*
1:45 Paper 471f: Deep Learning for Characterizing the Structure of Three-Dimensional, Binary, Self-Assembled Colloidal Lattices — ***Jared O'Leary**, Runfang Mao, Jeetain Mittal, Ali Mesbah*
2:00 Paper 471g: Networks of Anisotropic, Magnetically-Polarized Colloidal Particles Reversibly Reconfigure Under the Influence of an External Magnetic Field — ***Matthew Dorsey**, Orlin Velev, Carol Hall*
2:15 Paper 471h: Self-Assembling of a Non-Additive Mixture of Patchy Particles with Engineerable Energetic and Entropic Interactions — ***Isabela Quintela Matos**, Fernando Escobedo*

2:30 Paper 471i: Linker-Mediated Assembly of Nanocrystal Gels — ***Michael Howard***, *Zachary Sherman, Adithya N Sreenivasan, Stephanie A. Valenzuela, Eric V. Anslyn, Delia Milliron, Thomas Truskett*

(472) Continuous Crystallization Processes

Wednesday, Nov 10, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 302

Meenesh Singh, Chair
Baron Peters, Co-Chair

Sponsored by: Crystallization and Evaporation

12:30: Welcoming Remarks
12:33 Paper 472a: High-Efficient Crystal Particle Manufacture Via Microscale Process Intensification Technology — ***Xiaobin Jiang***, ***Gaohong He***
12:54 Paper 472b: Breakage Facilitated Mixed-Suspension, Mixed-Product-Removal (MSMPR) Crystallization — ***Huayu Li***, *Yuantao Li, Fan Liu, Bing-Shiou Yang*
1:15 Paper 472c: Electrochemical Sensor-Integrated, Continuous Flow, Microfluidic Device for Real-Time Measurement of Supersaturation during Salt Screening — ***Paria Coliaie***, *Aditya Prajapati, Manish Kelkar, Marianne Langston, Chengxiang Liu, Neda Nazemifard, Daniel Patience, Dimitri Skliar, Nandkishor K. Nere, Meenesh Singh*
1:36 Paper 472d: Periodic Forcing Via Temperature Cycles: Model-Based Study of Novel Continuous Configurations for Deracemization — ***Brigitta Bodák***, *Marco Mazzotti*
1:57 Paper 472f: Continuous Flow Synthesis of the Metal-Organic Framework HKUST-1 in a Millifluidic Reactor — ***Rajasi Shukre***, *Thomas Ericson, Anthony F. Cozzolino, Chau-Chyun Chen, Siva A. Vanapalli*
2:18 Paper 472g: Controlling the Effect of Slug-to-Slug Variation on the Crystal Size Distribution of Perovskite QDs: A CFD-Based Approach — ***Niranjan Sitapure***, *Robert Epps, Milad Abolhasani, Joseph Kwon*

(473) Conversion of Waste Plastic into Liquid Fuels

Wednesday, Nov 10, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 200

Shelby Browning, Chair
Jeffrey Seay, Co-Chair

Sponsored by: Waste Plastics

12:30 Paper 473a: *Chemical Upcycling of Waste Polyolefinic Plastics to Low-Carbon Synthetic Naphtha for Closing the Plastic Use Loop* — ***Leilei Dai Sr.***, *Nan Zhou, Paul Chen, Roger Ruan Sr.*
12:55: Break
1:20 Paper 473d: Deconstruction of Waste Polyethylene into Liquid Hydrocarbon Fuels and Lubricants over Ru Catalyst — ***Hongfei Lin***

(474) CO2 Industrial, Engineering and R&D Approaches II

Tuesday, Nov 16, 8:00 AM
Virtual, Environmental Division (09)

Xiaonan Wang, Chair
Selen Cremaschi, Co-Chair
Adam Usadi, Co-Chair

Sponsored by: Sustainability

8:00 Paper 474a: Electrospun Ca_2CuO_3 Fibrous Sorbent for Post-Combustion CO_2 Capture — ***Ehsan Hassani***, *Farshad Feyzbar-khalkhali-Nejad, Ali Rashti, Tae-Sik Oh*
8:25 Paper 474b: Steady State Flow Model for Impure CO2 Transportation in Industrial Processes — *Miguel Delgado*, ***Mariano Martin***
8:50 Paper 474c: Development of an Integrated System for Electrochemical CO_2 Capture and Conversion — ***Rohan Sartape***, *Aditya Prajapati, Meenesh Singh*
9:15: Break
9:40 Paper 474e: CO_2 Capture Using Phase-Changing Bis-Iminoguanidines (BIGs) with Amino Acids — ***Abishek Kasturi***, *Sotira Yiacoumi, Jorge Gabitto, Costas Tsouris, Diana Stamberga, Radu Custelcean*

(475) Data-Driven and Hybrid Modeling for Decision Making II

Wednesday, Nov 10, 12:30 PM
Sheraton Back Bay, Independence Ballroom East

Qi Zhang, Chair
Zhihong Yuan, Co-Chair

Sponsored by: Information Management and Intelligent Systems

12:30 Paper 475a: Multi-Objective Optimization Experimental Design Using a Exploration-Exploitation Trade-Off — ***Panagiotis Petsagkourakis***, *Federico Galvanin*
12:45 Paper 475b: Multi-Objective Bayesian Optimization of Process Flowsheets Using Trust Regions and Quality Set Metrics. — ***Edgar Sanchez Medina***, *Daniel F. Rodriguez-Vallejo, Antonio del Rio Chanona, Kai Sundmacher, Panagiotis Petsagkourakis*
1:00 Paper 475c: Formulation of Closed-Form Mathematical Expressions Applied to Chemical Engineering Processes Using the Bayesian Machine Scientist — ***Valentina Negri***, *Daniel Vázquez, Roger Guimerá, Marta Sales-Pardo, Gonzalo Guillén-Gosálbez*
1:15 Paper 475d: Data Clustering-Based Hybrid-Kinetic Model of an Industrial-Scale Biochemical Fermenter — ***Parth Shah, Masters***, *M. Ziyan Sheriff, PhD, Mohammed Saad Faizan Bangi, Joseph Kwon, Costas Kravaris*
1:30 Paper 475e: Optimization of Process Flowsheets Via Relu Neural Networks and Mixed-Integer Programming: Application to the Production of Green Ammonia. — *Panagiotis Petsagkourakis*, ***Andres Gonzalez***, *Antonio del Rio Chanona, Nilay Shah*
1:45 Paper 475f: A Hybrid Mechanistic-Machine Learning Approach for Identifying Governing Dynamical Equations of Algal Biodiesel Production Networks — *Raghav Moar, Shweta Singh*, ***Abhimanyu Raj Shekhar***
2:00 Paper 475g: Discovering Interpretable Models from Data Using Machine Learning: Application to Nonlinear Parametric Models — ***Arijit Chakraborty***, *Abhishek Sivaram, Venkat Venkatasubramanian*
2:15: Break

(476) Data-driven optimization

Wednesday, Nov 10, 12:30 PM
Sheraton Back Bay, Independence Ballroom West

Atharv Bhosekar, Co-Chair
Panagiotis Petsagkourakis, Co-Chair

Sponsored by: Systems and Process Operations

12:30 Paper 476a: *On the Use of Data Analytics Technology to Replace Dual Problems and Improve Decomposition Algorithms for Global Optimization Using Cutting Plane Approximations* — ***Asimina Marousi***, *Vasiliki Deligianni, Apostolos Chalkias, Antonios Kokosis*
12:49 Paper 476b: Deep Neural Network As Surrogates for Intractable Constraints and Problem Dimension Reduction: Security Constrained AC Optimal Power Flow — ***Zachary Kilwein***, *Jordan Jalving, Michael Eydenberg, Logan Blakely, Carl D. Laird, Fani Boukouvala*
1:08 Paper 476c: Optimization of Fischer-Tropsch Microchannel Reactor Using Computational Fluid Dynamics and Transfer-Learned Bayesian Optimization.— ***Kyoungmin Lee***, *Jong Min Lee*
1:27 Paper 476d: Computations and Optimization for Catalysts Under Dynamic Operation — ***Georgios Psarellis***, *Paul Dauenhauer, Mihalis Kavousanakis, Ioannis G. Kevrekidis*
1:46: Break
2:05 Paper 476f: Digitalizing the Process Industries Via Surrogate Optimization— ***Damien van de Berg***, *Tom Savage, Panagiotis Petsagkourakis, Nilay Shah, Damien van de Berg*
2:24 Paper 476g: Integration of Planning and Scheduling Using Data-Driven Feasibility Analysis — ***Oluwadare Badejo***, *Marianthi Ierapetritou*
2:43 Paper 476h: Training and Reformulating Neural Network Surrogate Models for Optimization — ***Calvin Tsay***, *Jan Kronqvist, Alexander Thebelt, Ruth Misener*

(477) Directed and Self Assembly of Colloids

Wednesday, Nov 10, 12:30 PM
Sheraton Back Bay, Back Bay Ballroom A

Ning Wu, Chair
Isaac Torres Diaz, Co-Chair

Sponsored by: Interfacial Phenomena

12:30 Paper 477a: Bioinspired Folding of Flexible Colloidal Polymers into Colloidal Materials — ***Angus McMullen***, *Jasna Brujic*
12:45 Paper 477b: Entropically Engineered Formation of Fivefold and Icosahedral Twin Clusters of Colloidal Shapes — ***Sangmin Lee***, *Sharon Glotzer*
1:00 Paper 477c: Assembly of Anisotropic Magnetized Particles — ***Thomas Thelen***, *Adriana Jara, Isaac Torres Diaz*
1:15 Paper 477d: Programming Interaction and Assembly with Magnetic Handshake Materials — ***Chrisy Xiyu Du***, *Hanyu Zhang, Tanner Pearson, Paul L. McEuen, Itai Cohen, Michael P. Brenner*
1:30 Paper 477e: Magnetic Control over Dynamic Clustering of Colloids— ***Bhuvnesh Bharti***, *Ahmed Al Harraq*
1:45 Paper 477f: Assembly of Magnetic Microspheres Under Combined Electric and Magnetic Fields — *Md Ashraful Haque*, ***Xingrui Zhu***, *Benjamin Hanson, Ning Wu*
2:00 Paper 477g: Coarse-Grained Modeling of Polarizable Nanoparticle Assembly — ***Siva Dasetty***, *Igor Coropceanu, Dmitri V. Talapin, Andrew Ferguson*
2:15 Paper 477h: Electric Field Mediated Assembly of Anisotropic Colloidal Particles — ***Michael Bevan***, *Rachel S. Hendley*
2:30 Paper 477i: The Stress in a Dispersion of Mutually Polarizable Spheres— ***Kelsey Reed***, *James Swan*
2:45 Paper 477j: Modification of the Pinning Properties of Interfacially Trapped Colloidal Ellipsoids Using External Electric Fields — ***Samuel Trevenen***, *Peter Beltramo*

(478) Emerging Junior Investigator Open Innovation Forum (Invited Talks)

Wednesday, Nov 10, 12:30 PM
Sheraton Back Bay, Republic Ballroom A

Jungwoo Lee, Chair
Eunsu Paek, Chair
Jinhye Bae, Co-Chair
Seok-Jhin Kim, Co-Chair
Yeongseon Jang, Co-Chair

Sponsored by: International Committee

12:30 Paper 478a: The Synergy between Experiment and Theory in Catalysis Research — ***Stephanie Kwon***
12:50 Paper 478b: Photoelectrochemistry of Semiconducting Polymers: Engineering Electronic Properties and Charge Carrier Dynamics — ***Won Tae Choi***
1:10 Paper 478c: Dynamics of Wetting Transitions in Complex Systems— ***Dongjin Seo***
1:30 Paper 478d: 3D Trajectories, Diffusion, and Interactions of Single Ceria Particles on a Glass Surface and Their Removal in Post-CMP Applications— ***Jihoon Seo***
1:50 Paper 478e: Robust Interfacial Tension Measurement and Surfactant Formulation Evaluation Protocol for Enhanced Oil Recovery — ***Jaeyub Chung***
2:10: Hanwha Travel Award Flash Presentations

(479) Engineering Drug Delivery Strategies and Biomolecular Sensors

Wednesday, Nov 10, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 108

Sijin Li, Co-Chair
Rong Tong, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

12:30 Paper 479a: DNA Aptamer-Decorated Gold Nanoparticles for *In Vivo*Detection of Human Matrix Metalloproteinase-9 Via Molecular Photoacoustic Imaging — ***Jinhwan Kim***, *Anthony Yu, Kelsey P. Kubelick, Stanislav Y. Emelianov*
12:48 Paper 479b: Investigating and Profiling the Engineering Potential of a Salicylic Acid Biosensor in *Escherichia coli* — ***Yusong Zou***, *Chenyi Li, Tian Jiang, Ruihua Zhang, Jian Wang, Yajun Yan*
1:06 Paper 479c: Development of a Delivery Strategy for Bioactive Albumin to Aid Bone Regeneration — *Stephanie Haag, Nathan Schiele,* ***Matthew Bernards***
1:24 Paper 479d: Design and Implementation of a Glucose-Responsive Genetic Switch Circuit in a Cell-Free System — ***Abhinav Adhikari***, *Jeffrey D. Varner*
1:42 Paper 479e: Engineering of Drug Formulations for the Prevention of Pre-Term Birth — ***Rachel Shapiro***, *Hannah Zierden, Kevin DeLong, Jairo I. Ortiz, Justin Hanes, Laura Ensign*
2:00 Paper 479f: Engineered Probiotics for Specific Sensing of Aromatic Amino Acids and Neurochemicals — *Austin Rottinghaus, Chenggang Xi, Matthew Amrofell, Hyojeong Yi,* ***Tae Seok Moon***
2:18 Paper 479g: Light and Metabolite Biosensors to Study and Engineer Cellular Metabolism (Invited Speaker) — ***Jose Avalos***

(480) Environmental Issues involving Biochar

Wednesday, Nov 10, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 308

Jeffrey Seay, Chair
Alvaro Orjuela, Co-Chair

Sponsored by: Sustainability

12:30 Paper 480a: Application of Waste Hay-Derived Biochar for Adsorption of Cyanobacterial Toxin in Water — *Yong-Keun Choi, Lu Ki Ong,* ***Eunsung Kan***
12:45 Paper 480b: Electro-Enhanced Removal of Heavy Metal Ions from Aqueous Solutions By Capacitive Deionization Process Using Biochar-Based Electrodes — ***Kalyani Mer***, *Nosa Egiebor, Wendong Tao, Baharak Sajjadi, Gyu Leem*
1:00 Paper 480c: The Impact of Inorganics on the Production and Use of Biochars Made from Household Biowaste — ***Amanda Simson***, *Lionel Gilliar-Schoenenberger*

(481) Fundamentals of Catalysis and Surface Science I: Single Atoms & Alloys

Wednesday, Nov 10, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 207

Omar Abdelrahman, Chair
Weijian Diao, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

12:30 Paper 481a: Single-Atom Alloy Catalysts: Born in a Vacuum, Tested in Reactors, and Understood in silico — ***E Charles Sykes***
12:48 Paper 481b: Controlling Formic Acid Decomposition through Alloy and Ensemble Effects on PdCu Catalysts — ***Yu Liu***, *Saurabh Bhandari, Manos Mavrikakis, Konstantinos Goulas, Lars Grabow*
1:06 Paper 481e: Density Functional Theory (DFT) Analysis of C-H Bond Formation on Anatase TiO_2-Supported Single-Atom Catalysts — ***Jeremy Hu***, *Konstantinos Alexopoulos, Michael Janik*
1:24 Paper 481f: Universal Vibrational and Entropic Scaling Relationships for Dehydrogenations — ***Sophia Kurdziel***, *Joshua Lansford, Dionisios Vlachos*
1:42 Paper 481g: Kinetic Description of Site Ensembles on Catalytic Surfaces— ***Neil Razdan***, *Aditya Bhan*

(482) How to Share Your Research with Everyone

Wednesday, Nov 10, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 312

Shelby Mills, Chair

Sponsored by: Young Professionals Committee (YPC)

(483) Immunoengineering

Wednesday, Nov 10, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 109

Laurel Hind, Co-Chair
Kayla Sprenger, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

12:30 Paper 483a: Understanding a Highly Microparticle Sensitive, Temporally Controlled Dendritic Cell Subset: Implications for Improving Vaccines — ***Peter Deak***, *Bradley Studnitzer, Aaron Esser-Kahn*
12:48 Paper 342be: RBD Escape Mutations Span Multiple Antibodies — ***Emily Rhodes***, *Tim Whitehead, Kayla Sprenger*
1:06 Paper 483c: Engineering Immunoinstructive Cryogel Scaffolds to Induce Regulatory T-Cells — *Loek Eggermont,* ***Thibault Colombani***, *Christopher Meehan, Johanna Wilson,* ***Sidi A Bencherif***
1:24 Paper 483d: Engineering Metabolically Armored T Cell Therapies for Solid Tumor Translation — ***John Cox***, *John Blazeck*
1:42 Paper 483e: Unraveling the Crosstalk between Neutrophils, Platelets, and Extracellular Vesicles in Breast-to-Lung Metastasis — ***Hunter Snoderly***, *Olivia Miller, Abby Ivey, Brian Boone, Margaret Bennewitz*
2:00 Paper 483f: Navigating the Matrix: How Neutrophils Interact with Their Microenvironment — ***Christopher Calo***, *Isaac Richardson, Laurel Hind*
2:18 Paper 483g: Programming Immunity with Smart Materials (Invited Speaker) — ***John Wilson***

(485) Innovations in Concept-to-Manufacturing and Distribution I

Wednesday, Nov 10, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 201

Xiaonan Wang, Chair
Alexander Dowling, Co-Chair

Sponsored by: Next-Gen Manufacturing

12:30 Paper 485a: Integrated Design and Model Predictive Control of Multiscale Systems Using a Multi-Fidelity Bayesian Optimization Approach — *Farshud Sorourifar, Naitik A. Choksi,* ***Joel Paulson***
12:50 Paper 485b: Adjustable Robust Optimization for the Planning Operations of Integrated Refinery-Petrochemical Site Under Demand Uncertainty — ***Zhang Lifeng***, *Zhihong Yuan, Bingzhen Chen*
1:10 Paper 485c: A Novel Hybrid Algorithm for Scheduling of Multipurpose Batch Process — ***Dan Li***, *Dongda Zhang, Nan Zhang, Jie Li, Liping Zhang, Xin Xiao*
1:30 Paper 485d: Impact of Split Delivery in Minimizing LNG Procurement Cost— ***Prashanth Ravula***, ***Mohd Shahrukh***, ***Rajagopalan Srinivasan***, ***Iftekhar Karimi***
1:50 Paper 485e: Keynote Talk: Toward Autonomy for Safe and on-Demand Biomanufacturing on Mars — ***Ali Mesbah***
2:25 Paper 485f: Keynote Talk: The Roadmap to an Autonomous Chemistry Lab— ***Connor Coley***

(486) Integrated Design of Drug Product Formulation, Manufacture and Delivery

Wednesday, Nov 10, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 101

Shujauddin Changi, Co-Chair
Pablo Rolandi, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

12:30 Paper 486a: Exploring the Physical Aging Behavior of Hpmcas *Via*Thermal Analysis — ***Yejoon Seo***, *Rodney Priestley*
12:54 Paper 486b: Accurate Temperature Prediction of the Freeze-Dried Cake during Secondary Drying Process in a Laboratory Scale Lyophilizer — ***Kyu Yoon***, *Vivek Narsimhan*
1:18 Paper 486c: Physicochemical Modeling of Drug Stability in Multilayer Polymeric Films Containing an Aqueous Moisture Barrier Layer — ***M. Arif Khan***, *Andie L. MacMillan, Aktham Aburub, Karthik Vaideeswaran, Sarah Clark, Mohamed ElSayed, Shekhar K. Viswanath, Thomas D. Dziubla*
1:42 Paper 486f: Development of an HME Based Extended-Release Formulation Using Experimental and in silico Approach — ***Josip Matic***, *Varun Kushwah, PM Martinez, Estelle Beguin, Manjeet Pimparade, Jeff Katstra, Amrit Paudel, Johannes G. Khinast*

(487) Membrane Modeling and Simulation

Wednesday, Nov 10, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 304

Xianghong Qian, Co-Chair
Nitish Mittal, Co-Chair

Sponsored by: Membrane-Based Separations

12:30 Paper 487a: Bypass in Hollow Fiber Gas Separation Membrane Modules— *Lili Sun, Grigorios Panagakos,* ***Glenn Lipscomb***
12:45 Paper 487b: Separation of Organic Solvents Using Dual-Layer Hollow Fiber Mixed Matrix Membranes — ***Conrad Roos***, *Hye Youn Jang, Yao Ma, Ryan Lively*
1:00 Paper 487c: Modeling and Simulation of Gas Separations with Spiral-Wound Membranes — ***Robert DeJaco***, *Ken Loprete, Kenneth J. Pennisi, Sudip Majumdar, Joern Siepmann, Prodromos Daoutidis, Hannah Murnen, Michael Tsapatsis*
1:15 Paper 487d: Generalized Synthesis of Membrane Systems for Multicomponent Gas Separation — ***Garry Taifan***, *Christos Maravelias*
1:30 Paper 487e: Predicting Molecular Diffusion in Flexible Metal Organic Frameworks — ***Yuhan Yang***, *David Sholl*
1:45 Paper 487f: A Theoretically Self – Consistent Netgp Approach for the Solubility of Vapors and Liquids in Glassy Polymers Based on the Perturbation of a Dry Glassy Reference State — ***Bennett Marshall***, *Ronita Mathias, Ryan Lively, Benjamin A. McCool*

(488) Membranes for Electrochemical Conversions and Applications I

Wednesday, Nov 10, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 301

Winston Ho, Co-Chair
Peter N. Pintauro, Co-Chair

Sponsored by: Membrane-Based Separations

12:30 Paper 488a: New Developments in Polybenzimidazole (PBI) Membranes for Electrochemical

Devices — ***Brian Benicewicz***, *Fei Huang, Laura Murdock*
1:00 Paper 488b: Ion Pair Polymer Membranes for High Temperature Proton Exchange Membrane Fuel Cells — ***Yu Seung Kim***
1:30 Paper 488d: Structure-Property Relationships in Highly Permeable Dioxolane-Based Perfluorinated Ionomers with Tunable Transport Properties — *Adlai Katzenberg, Yoshiyuki Okamoto, Ahmet Kusoglu,* ***Miguel Modestino***
2:00 Paper 488f: Poly(Phenylenesulfonic Acid)-Based PEMs for Low RH Fuel Cell Operation — *Zhihao Shang, Mohammad Hossain, R. Wycisk,* ***Peter N. Pintauro***

(489) Metabolic Engineering for Food, Feed, and Bioproducts

Wednesday, Nov 10, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 107

Jie Dong, Chair
Teng Bao, Co-Chair
Ting Lu, Co-Chair

Sponsored by: Food

12:30 Paper 113g: [Invited Keynote] Biorefinery for Carboxylic Acids Production from Renewable Biomass — ***Shang-Tian Yang***
1:10 Paper 489b: Biodegradable Polyhydroxyalkanoate Production from Plasma Oxidized Non-Degradable Polypropylene — ***Logan Mushill***, *Mohammad Shahinur Rahaman, Noppadon Sathitsuksanoh, Jie Dong*
1:28 Paper 489e: Metabolic Engineering of *Aureobasidium Pullulans* for Enhanced Polymalic Acid Production through Enhancing Oxaloacetate Conversion, Malate Transportation, and PMA Synthesis — ***Zhen Qin***, *You Li, Yin Zheng, Shang-Tian Yang*
1:46 Paper 113d: Engineering of Fast Growing Cyanobacteria *Synechococcus Elongatus* sp. PCC 11801 for Phenylalanine Production — ***Arnav Deshpande***, *John A. Morgan*
2:04 Paper 489g: [Invited Keynote] Engineering a Microbial Cooperative Consortium for Chemical Production — ***Ting Lu***

(490) Microfluidic and Microscale Flows: Multiphase and Fields

Wednesday, Nov 10, 12:30 PM
Sheraton Back Bay, Constitution B

Qin Qi, Chair
Jeffrey Richards, Co-Chair

Sponsored by: Fluid Mechanics

12:30 Paper 490a: Temperature Dependence of Diffusiophoresis Using a Novel Microfluidic Approach. — ***Parth Shah***, *Huanshu Tan, David Taylor, Xiaoyu Tang, Afnan Mashat, Nan Shi, Amr Abdel-Fattah, Todd Squires*
12:45 Paper 490b: Flow Behavior of Chiral Liquid Crystals — *Sepideh Norouzi, Mohsen Esmaeili, Jose A. Martinez-Gonzalez, Nader Taheri-Qazvini, Rui Zhang,* ***Monirosadat Sadati***
1:00 Paper 490c: Learning Hidden Rheology Using Rheology-Informed Graph Neural Networks (RhIGNets) — *Mohammadamin Mahmoudabadbozchelou,* ***Safa Jamali***
1:15 Paper 490d: Liquid Handling Strategies for X-Ray Compatible Microfluidics— ***Sarthak Saha***, *Shuo Sui, Sarah L. Perry*
1:30 Paper 490e: Detecting Molecules with an Electrokinetic Instability in Membrane Microfluidics — ***Hsueh-Chia Chang***, *Satyajyoti Senapati, Sebastian Sensale, Zeinab Ramshani*
1:45 Paper 490f: High Shear Microstructure and Rheology of Rod-like Viruses Via Capillary Rheo-SANS — ***Steve Kuei***, *Paul F. Salipante, Ryan P. Murphy, Katie Weigandt, Steven D. Hudson*
2:00 Paper 490g: Experimental Two-Phase Fluid Displacement in Microchannels with Pure Viscoelastic Fluids — ***Seng Hoe Hue***, *Panagiota Angeli*
2:15 Paper 490h: Non Newtonian Fluid Flow through Converging Diverging Channel — ***Garima Vishal***, *Sudip Pattnayek, Jayati Sarkar*
2:30 Paper 490i: Ternary Fluid Lattice Boltzmann Simulation of Dynamic Interfacial Tension Induced By Mixing inside Micro-Droplets — ***Hao Wang***, *Yi Cheng*
2:45 Paper 490j: Giant Unilamellar Vesicle Dynamics in Oscillatory Extension— ***Charlie Lin***, *Dinesh Kumar, Channing Richter, Shiyan Wang, Charles M. Schroeder, Vivek Narsimhan*

(491) Modeling and Analysis of Chemical Reactors II

Wednesday, Nov 10, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 206

Nitish Mittal, Chair
Eric Moschetta, Co-Chair
Xinrui Yu, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

12:30 Paper 491a: Transverse Pattern Formation Analysis with Cell Model— ***Meet Shah***, *David West, Vemuri Balakotaiah*
12:55 Paper 491b: An Open-Source Library for Multi-Step Reactions in Spherical and Cylindrical Particles — ***John Wakefield***, *Aaron Lattanzi, M. Brennan Pecha, Peter N. Ciesielski, Jesse Capecelatro*
1:20: Break
1:45 Paper 491d: Analysis of Wall Shear Stress and Velocity Gradient from Fluid Flow on a Microreactor System — ***James Morris***, *Zhenzhen Xie, Xiao-an Fu, R. Eric Berson*
2:10 Paper 491e: Simulation of the Diffusion-Limited Deposition of Diethylzinc in a Mesoporous Alumina Substrate — *Liwei Zhuang,* ***Peter Corkery***, *Dennis Lee, Michael Tsapatsis*
2:35 Paper 491f: Multi-Scale Analysis of Chemical Reactors Using Green's Function Method — ***Dharmendra Mandaliya***, *Ravindra D. Gudi*

(492) Modeling, Control, and Optimization of Energy Systems I

Wednesday, Nov 10, 12:30 PM
Sheraton Back Bay, Back Bay Ballroom D

Corey James, Chair
Calvin Tsay, Co-Chair

Sponsored by: Systems and Process Control

12:30 Paper 492a: Industrial Battery Storage Dispatch and Optimization Using Gaussian Process Regression and Bayesian Decision Theory — ***Blake Billings***, *Philip Smith, Sean Smith, Kody Powell*
12:49 Paper 492b: Optimal Resource Allocation in a Subsea Oil Production Network Using Distributed Feedback-Based RTO — ***Risvan Dirza***, *Sigurd Skogestad, Dinesh Krishnamoorthy*
1:08 Paper 492c: A Computational Approach to Enhance the Economic Viability of Acid Fractionation Via Multiscale Modeling and Economic Model Predictive Control — ***Hyun-Kyu Choi***, *Chang Geun Yoo, Joseph Kwon*
1:27 Paper 492e: Dynamic Optimization of the Operational Trajectory of a Supercritical Pulverized Coal-Fired Boiler Under Load-Following with Consideration of Boiler Health — ***Katherine Reynolds***, *Elijah Hedrick, Benjamin P. Omell, Stephen E. Zitney, Debangsu Bhattacharyya*
1:46 Paper 492f: Nonlinear Model Predictive Control Simulations of Gas-Solid Reactors for Chemical Looping Combustion of Methane — ***Robert Parker***, *Lorenz Biegler*
2:05 Paper 492g: Decision Support Software for Optimal Decarbonisation Policymaking for Carbon Constrained Growth in Developing Countries – a Malaysian Case Study — *Purusothmn N.S.B. Nair,* ***Michael Short***, *Matteo Cossutta, Jully Tan, Yasunori Kikuchi, Raymond R. Tan, Dominic Chwan Yee Foo*
2:24 Paper 492h: Model Predictive Control for Energy Scheduling of Pipeline Networks — ***Lu Zhang***, *Junyao Xie, Stevan Dubljevic*

(493) Next Generation Biomolecules and Bioprocesses

Wednesday, Nov 10, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 303

Christoph Brandenbusch, Chair
Maximilian Wessner, Co-Chair

Sponsored by: Bio Separations

12:30 Paper 493a: Factors Affecting Robustness of Anion Exchange Chromatography: Selective Retention of Minute Virus of Mice Using Membrane Media — *Shu-Ting Chen, Wenbo Xu, Ranil Wickramasinghe, Kang Cai, Gisela Ferreira,* ***Xianghong Qian***
12:48 Paper 493b: Towards Cost-Effective Downstream Processes for the Purification of Therapeutic Viruses — ***Karina Kawka***, *Shayna Earle, Ian Gough, Nicholas Graham, Yuki Abe, Maria Fe C. Medina, Brian Lichty, Raja Ghosh, David Latulippe*
1:06 Paper 493c: Model-Based Control for Column-Based Continuous Viral Inactivation of Biopharmaceuticals — ***Moo Sun Hong***, *Amos E. Lu, Rui Wen Ou, Jacqueline Wolfrum, Stacy Springs, Anthony J. Sinskey, Richard Braatz*
1:24 Paper 493d: A Membrane-Based Purification Platform for Plasmid-DNA Production — *Jialiang Huang, Cindy Saliba, Peter Levison, Leticia Reyes-Regis, Michael Mitchell, Chris Tseng, Julie Pressman, Andria Balogh,* ***Saurav Datta***, *Hu Zhang*
1:42 Paper 493e: Development of Nanopocket Membranes for the Purification and Fractionation of Extracellular Vesicle Subpopulations — ***Thomas Gaborski***, *Mehdi Dehghani, Shayan Gholizadeh, Munther Alsudais*
2:00 Paper 493f: Rapid, High Throughput mRNA Purification. — ***Jinxiang Zhou***, *Graham Temples*
2:18 Paper 493g: Characterization of Sedimentation and Filtration of Mechanically Labile Protein Crystals on a Small Scale — ***Benjamin Radel***, *Hermann Nirschl*
2:36 Paper 493h: Supramolecular Engineering of Self-Assembling High Affinity Polymers for Binding-Triggered Phase Separation and Antibody Purification— ***David Stern***, *Yi Li, Lye Lin Lock, Jason Mills, Xuankuo Xu, Sanchayita Ghose, Zheng Jian Li, Honggang Cui*

(494) Next-Gen Manufacturing in Pharma, Food, and Bioprocessing I

Wednesday, Nov 10, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 202

Manjiri Moharir, Chair
Maria Papathanasiou, Co-Chair

Sponsored by: Next-Gen Manufacturing

12:30 Paper 494a: Multi-Objective Supply Chain Optimization in Personalized Healthcare — ***Andrea Bernardi***, *Niki Triantafyllou, Athanasios Antonakoudis, Matthew Lakelin, Nilay Shah, Maria Papathanasiou*
12:53: Break
1:18 Paper 494c: Robust Bioprocessing of Lignocellulose Using Microbial Tipping Points — ***Katharine Hirl***, *Michael J. Shreve, John M. Regan, Tom L. Richard*
1:41 Paper 494d: Keynote: Multi-Objective Optimization, State Estimation, and Advanced Control of a Semi-Batch Process for the Enzymatic Conversion of Lactose into Value-Added Products — ***Ronald Alexander***, *San Dinh, Guilhermina Schultz, Marcelo P. A. Ribeiro, Fernando V. Lima*
2:16 Paper 494e: Keynote: Virtual-Engineering Software Framework for Integrated Biomass Conversion Modeling — ***Ethan Young***, *Hariswaran Sitaraman, Andrew Glaws, Andrew Bartling, James J. Lischeske, Jonathan Stickel*

(495) Nitrogen Chemistry II: N2 Reduction

Wednesday, Nov 10, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 203

Meenesh Singh, Chair
Joseph Gauthier, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

12:30 Paper 495a: Chemical Looping Synthesis of Ammonia over Cobalt Molybdenum Nitride: Effects of Surface Hydrogen on Productivity — ***Sean Brown***, *Jianli Hu*
12:50 Paper 495b: Performance Targets for Renewable Electricity-Based Electrochemical Ammonia Production — ***Nikifar Lazouski***, *Michal Gala, Abhishek Bose, Karthish Manthiram, Dharik Mallapragada*
1:10 Paper 495c: Microwave-Enhanced Catalytic Ammonia Synthesis over Csru/CeO_2 Under Moderate Pressure and Temperature — ***Yuxin Wang***, *Alazar Araia, Xinwei Bai, Christina Wildfire, Dushyant Shekhawat, Debangsu Bhattacharyya, Tuhin Suvra Khan, Jianli Hu*
1:30 Paper 495d: Mechanocatalytic Ammonia Synthesis over Transition Metal Nitrides — ***Karoline L. Hebisch***, *Andrew Tricker, Erin V. Phillips, Marco Buchmann, Yu-Hsuan Liu, Marcus Rose, Eli Stavitski, Andrew Medford, Marta Hatzell, Carsten Sievers*
1:50 Paper 495e: Electric Fields Accelerated Nitrogen Chemistry — ***Fanglin Che***

(496) Optoelectronic Materials Theory, Microscopy, and Spectroscopy

Wednesday, Nov 10, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 104

Yuzhang Li, Chair

Sponsored by: Electronics and Photonics

12:30 Paper 496a: Photophysical Characterization of New Intrinsic Charge Transfer States in Proteins — ***Leah Spangler***, *Michael H. Hecht, Gregory D. Scholes*
12:45 Paper 496b: Optoelectronic Properties of Graphene-Noble Metal Thin Films for Energy Storage and Conversion Applications — ***Enoch Nagelli***, *Jeffrey Chin, Taylor Vessel*
1:00 Paper 496c: Instrumentation and Strategies for Hyperpolarized NMR Spectroscopy — ***Kaitlyn Engler***, *Jeffrey A. Reimer, Jeffrey R. Long*
1:15 Paper 496d: Tight-Binding Model Accurately Describes Frontier Orbitals of Conjugated Oligomer Acceptors for Organic Solar Cells — ***Vishal Jindal***, *Puja Agarwala, Michael J. Janik, Scott T. Milner*
1:30 Paper 496e: Effect of Substrate, Polarization, and Orientation on the Scattering Behavior of Differently Shaped Individual Gold Nanostructures — ***Md Monirul Islam***, *Md Mir Hossen, Thomas Koschny, Andrew C. Hillier*
1:45 Paper 496f: Quantifying the Accuracy and Uncertainty in Back Focal Plane Imaging for Nanostructured Materials and Optoelectronics — *Tung-Tung Lin,****Carissa Eisler***
2:00 Paper 496g: Nanostructure Pattern Formation in Epitaxially Grown Strained Semiconductor Thin Films As an Outcome of a Nonlinear Surface Morphological Instability — ***Chao-Shou Chen***, *Ashish Kumar, Dimitrios Maroudas*

(497) Particle Technology Forum Award Presentations and Baron Award Lecture (Invited Talks)

Monday, Nov 15, 3:30 PM
Virtual, Particle Technology Forum (03)

Ben Freireich, Chair

Sponsored by: Particle Technology Forum

3:30 Paper 497a: Thomas Baron Award in Fluid-Particle Systems (Sponsored by Shell): Design of Multiphase Reactors for the Synthesis of Renewable Chemicals and Semiconductor Nanocrystals — ***Triantafillos Mountziaris***
4:15 Paper 497b: Elsevier Lifetime Achievement Award: Fluidization Centennial -- Reflection on the Past and Prospection in the Future — ***Jesse Zhu***
5:00 Paper 497c: PSRI Lectureship Award in Fluidization: CFD as a tool to better understand multiphase flow physics — ***Sofiane Benyahia***

(498) Particulate and Multiphase Flows: Emulsions, Bubbles, Droplets

Wednesday, Nov 10, 12:30 PM
Sheraton Back Bay, Constitution A

Ryan Poling-Skutvik, Chair
Samanvaya Srivastava, Co-Chair

Sponsored by: Fluid Mechanics

12:30 Paper 498a: Tuning the Yield Stress in Suspensions of Soft Colloids— ***Ryan Poling-Skutvik***, *Daniel Keane, Abhishek Dhand*
12:45 Paper 498b: The Effects of Suspending Fluid Viscoelasticity on Red Blood Cell Dynamics — *Mehdi Niazi Ardekani,* ***Boon Siong Neo***, *Eric Shaqfeh*
1:00 Paper 498c: The Effect of Particle Characteristics on the Hydrodynamic Separation of Binary Systems — ***Sabrina Marnoto***, *Sara Hashmi*
1:15 Paper 498d: Impact of Surface Viscosity on the Stability of a Droplet Translating through a Stagnant Fluid — ***Vivek Narsimhan***, *Natasha Singh*
1:30 Paper 498e: Elliptical Pipette Generated Droplets for Digital PCR Quantification of Saliva Viral Load — ***Liao Chen***, *Vivek Yadav, Hsueh-Chia Chang*
1:45 Paper 498f: Stretch, Fold, and Break: Intensification of Emulsification of High Viscosity Ratio Systems By Fractal Mixers — ***Martin Hofmann***, *Alexandra V. Bayles, Jan Vermant*
2:00 Paper 498g: Numerical Investigation of Deformable Drops in Three-Dimensional Microchannels Using a Moving-Frame Boundary-Integral Method— ***Gesse Roure***, *Robert Davis, Alexander Zinchenko*
2:15 Paper 498h: Numerical Investigation of Enhanced Dehumidification Processes By Using Dilectrophoresis Principles in Moist Airflows — *Maliha Yel Mahi, Yasuhiro Shoji,* ***David Young***, *Selen Cremaschi, Lorenzo Cremaschi*
2:30 Paper 498i: Effect of Additives to the Droplet Impact Dynamics — ***Xiaoyu Tang***

(499) Policy and Sustainability

Wednesday, Nov 10, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 313

Ashley Pennington, Chair
Gerardo Ruiz-Mercado, Co-Chair
Jason Trembly, Co-Chair

Sponsored by: Sustainable Energy

12:30 Paper 499a: Addressing the Socio-Economic Disparities of Net Zero Transition — ***Piera Patrizio***, *Pratama Yoga Wienda, Niall Mac Dowell*
12:45 Paper 499b: Decarbonising Residential Heating: Cost-Benefit Analysis to Support Policy Design — ***Jennifer Penman***, *Sheila Samsatli*
1:00: Break
1:15 Paper 499d: How Policy Can Enable Domestic Energy Transformations: A Lesson from LNG — ***Michael Stern***, *Achim Wechsung, Michael Orella, Sandra Safro, Elizabeth Crouse, Harri K. Kytömaa*
1:30 Paper 499e: Over Half a Century of Protecting the Environment through Various Policies, Administrations, Successes, & Failures; An Overview of 50+ Years of EPA Regulations and Standards — *Ashley Pennington,* ***Robert Peters***
1:45 Paper 499f: Improving the Economics of Industrial Battery Storage: A Proactive Policy and Management Approach — ***Blake Billings***, *Anne Dougherty, Nestor Camacho, Kody Powell*

(500) Polymer Simulations 1: Method and Theory

Wednesday, Nov 10, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 209

Douglas Tree, Chair
Poornima Padmanabhan, Co-Chair

Sponsored by: Polymers

12:30 Paper 500a: At the Nexus of Simulation and Machine Learning for Sequence Design of Polymers — ***Michael Webb***
1:00 Paper 500b: Combined Equation of State Modelling and Coarse-Grained Molecular Simulation of Polymers and Polymer Mixtures Via SAFT-γ Mie— ***Maziar Fayaz Torshizi***, *Erich A Muller*
1:15: Break
1:30 Paper 500d: An Implicit Approach for Simulating Strongly Directional Interactions — ***Dong Meng***, *Jing Zong*
1:45 Paper 500e: Stochastic Kinetic Theory Applied to Nonequilibrium Polymer Simulations — ***Patrick Underhill***
2:00 Paper 500f: Automated Multiscale Simulations for Materials Discovery— ***Ludwig Schneider***, *Marcus Schwarting, Joshua Mysona, Phillip Rauscher, Heyi Liang, Ming Han, Phwey Gil, Juan J. de Pablo*
2:15 Paper 500g: A Multiscale Pipeline for Polymer Network Design and Mechanical Property Prediction with Reaction Detection — ***Nathan Rebello***, *Tzyy-Shyang Lin, Bradley Olsen*
2:30 Paper 500h: Self-Avoiding Random Walks Generated By Iterated Function Systems — ***Glenn Lipscomb***
2:45 Paper 500i: Thermal Barrier Coatings for Cellulose Substrates: A Designed Molecular Simulation Study of the Effects of Nanoparticles and Porosity on Thermal Diffusivity — *Mohammad Mansourian-Tabaei, Alireza Asiaee, Brenda Hutton-Prager,* ***Sasan Nouranian***

(501) Practical Applications of Computational Chemistry and Molecular Simulation II

Wednesday, Nov 10, 12:30 PM
Marriott Copley Place, Salon J/K

Martin Sanborn, Chair
Steven G. Arturo, Co-Chair
Andrea R. Browning, Co-Chair
Jonathan Moore, Co-Chair
Phillip Westmoreland, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

12:30 Paper 501a: Determining Optimal Solvents for High-Throughput Processing of Extreme-Strength Covalent Organic Frameworks — *Emily Rankin, Emily Borza, Emil Sandoz-Rosado, Poornima Padmanabhan,* ***Obioma Uche***
12:50: Panel Discussion
1:10 Paper 501c: Computational Modeling of Aluminum Covetics for Improving Manufacturing Yields — ***Devyesh Rana***, *Steven Lustig*
1:30 Paper 501d: Molecular Aspects of Temperature Swing Solvent Extraction for Brine Desalination Using Imidazole-Based Solvents. — ***Gabriel Barbosa***, *Jason Bara, Steven Weinman, C. Heath Turner*
1:45 Paper 501e: Quantitative Characterization of Modern CO2-Absorbent Ionic Liquids Using Molecular Dynamics Simulation with the Interface Force Field— ***ISAAC Armstrong***, *Hendrik Heinz*
2:00 Paper 501f: Brownian Bridge Method for Studying Rare Events – an Approximation Scheme — ***Shiyan Wang***, *Anirudh Venkatesh, Pelin Su Bulutoglu, Doraiswami Ramkrishna, Vivek Narsimhan*
2:15: Panel Discussion
2:30 Paper 501h: Development of Two Sequential Kmc Models to Describe Ligand Exchange and Charge Transport for $CsPbBr_3$ Quantum Dots with Improved

Stability and Charge Carrier Mobility — ***Jiwon Roh***, *Niranjan Sitapure, Sang Hwan Son, Il Moon, Hyungtae Cho, Joseph Kwon, Junghwan Kim*
2:45 Paper 501i: Mechanism of Inorganic Phosphate Release Reaction in Actin Subunits — ***Sriramvignesh Mani***, *Gregory A. Voth*

(502) Resilient and Sustainable Supply Chains and Product Systems

Tuesday, Nov 16, 8:00 AM
Virtual, Sustainable Engineering Forum (23)

Ashley Pennington, Chair
Vikas Khanna, Co-Chair
Simona Liguori, Co-Chair

Sponsored by: Sustainability Science and Engineering

8:00 Paper 502a: Resilience in the Face of COVID-19: Managing a User Program at the Molecular Foundry — ***Shannon Ciston***
8:25 Paper 502b: Global Supply Chain Optimization for COVID-19 Vaccines Under Covax Facility — ***Apoorva Katragadda***, *Xiaonan Wang, Iftekhar Karimi*
8:50 Paper 502c: Sustainability and Resiliency Assessment for Industrial Synergies between Renewable Energy and Chemical Production — ***Apoorva Bademi***, ***William Farlessyost***, ***Miriam Stevens***, *Shweta Singh*
9:15 Paper 502d: A Community-Level Energy Planning Model for the Dynamic Optimization of Waste-to-Gas and Waste-to-Power Anaerobic Digestion Supply Chains. — ***Irene Mas Martin***, *Alvina Aui, Lisa Schulte, Mark Mba Wright*
9:40 Paper 502e: Asset Integrity Management (AIM) for Hydrogen: Major Incident Risk Reduction By Integrating a Risk-Based Safety Approach — ***Gareth Ellor***
10:05 Paper 502f: More Haste, Less Speed: Proportionate Supply Chain Risk Management for the Accelerating Hydrogen Economy — ***Gareth Ellor***

(503) Survey Results and Best Practices (Invited Talks)

Wednesday, Nov 10, 12:30 PM
Sheraton Back Bay, Republic Ballroom B

Laura Ford, Chair
Janie Brennan, Co-Chair

Sponsored by: Undergraduate Education

12:30 Paper 503a: How We Teach: Survey Results for Material and Energy Balances — ***Laura Ford***
1:00 Paper 503b: MEB: The Sun in the Center of the ChE Universe — ***Lisa Bullard***
1:30 Paper 503c: Discussion: Issues and Best Practices in Teaching Material and Energy Balances — ***Janie Brennan***

(504) Sustainable Energy: Generation and Storage

Wednesday, Nov 10, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 310

Sheila Samsatli, Chair
Ashley Pennington, Co-Chair
Vilas G. Pol, Co-Chair

Sponsored by: Sustainable Energy

12:30 Paper 504a: Enabling Low Carbon Hydrogen Production Using Resource Integration Approach — ***Yasir Ibrahim***, *Dhabia Al-Mohannadi*
12:45 Paper 504b: The Effect of Geological Properties of Underground Storage on Its Suitability for Inter-Seasonal Storage of Hydrogen and Its Role in Achieving Net Zero — ***Natasha Marino***, *Jennifer Penman, Sheila Samsatli*
1:00 Paper 504c: Stone-Wales Defect-Rich Carbon-Supported Dual-Metal Single Atom Sites for Zn-Air Batteries — ***Kishwar Khan***, *Zhengtang Luo, Khalil Amine*
1:15 Paper 504d: Determination of Safety Parameters in Lithium-Ion Batteries— ***Surendra Singh***
1:30 Paper 504e: Silica Gel/ $MgSO_4$ Hybrids for Thermal Energy Storage— ***Subodhi Shervani***, *F Handan Tezel*
1:45 Paper 504f: Thermochemical Heat Recuperation for Compressed Air Energy Storage — ***Fuqiong Lei***, *Like Li, Eric Million, David Korba, Kelvin Randhir, Nick AuYeung*
2:00 Paper 504g: Exploring the Role and Value of Grid-Scale Energy Storage in Deep Decarbonisation — ***Caroline Ganzer***, *Yoga Wienda Pratama, Niall Mac Dowell*
2:15 Paper 749c: Data-Driven Incipient Fault Management for Proton Exchange Membrane Fuel Cell — ***Bhavana Bhadriraju***, *Joseph Kwon, Faisal Khan*

(505) Systems and Quantitative Biology: Disease Mechanisms, Biomarkers, and Therapies

Wednesday, Nov 10, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 111

Hyun-Seob Song, Chair
Kate Galloway, Co-Chair

Sponsored by: Bioengineering

12:30 Paper 505a: Clonally Expanded, GPR15-Expressing Pathogenic Effector Th2 Cells Are Associated with Eosinophilic Esophagitis — ***Duncan Morgan***, *Bert Ruiter, Neal Smith, Ang A. Tu, Brinda Monian, Brandon Stone, Navneet Virk-Hundal, Qian Yuan, Wayne G. Shreffler, J. Christopher Love*
12:48 Paper 505b: Single-Cell Analysis of Drug-Induced Proneural-to-Mesenchymal Transition in Patient-Derived GBM Stem-like Cells — ***James Park***, *Adrian Lopez Garcia de Lomana, Wei-Ju Wu, Parvinder Hothi, Charles Cobbs, Sui Huang, Nitin Baliga*
1:06 Paper 505c: Harnessing p53 to Stabilize Accelerated, Dual-Phase Reprogramming — ***Kate Galloway***
1:24 Paper 505d: Transcriptome and Methylome Analysis of Distal Spinal Cord Location after Spinal Cord Injury — ***Junkai Xie***, *Chongli Yuan, Han Zhao*
1:42 Paper 505e: Low-Input Technology Reveals Prolonged Epigenomic Alterations Following Single Exposure to a Psychedelic in Mice — ***Bohan Zhu***, *Mario de la Fuente Revenga, Lynette Naler, Justin M. Saunders, Zirui Zhou, Rudy Toneatti, Salvador Sierra, Chang Lu, Javier González-Maeso*
2:00 Paper 505f: Dermal Fibroblast Morphology and Collagen Fiber Alignment As Aging Biomarker. — ***Kyu Sang Han***, *Pei-Hsun Wu, Denis Wirtz*
2:18 Paper 505g: Compartmental Analysis of Redox Metabolism to Inform Therapeutic Strategies — ***Hadley D. Sikes***

(506) Teaching Data Science to Students and Teachers II

Wednesday, Nov 10, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 306

Martha Grover, Chair
Phillip Westmoreland, Co-Chair

Sponsored by: Bridging the Skills Gap in Chemical Engineering

12:30 Paper 506b: Insights from Teaching "Data Analytics for Chemical Engineers" — ***Andrew Medford***
1:00 Paper 506c: Tips and Pitfalls to Avoid When Teaching Machine Learning with Python to Chemical Engineering Students at the Undergraduate and Graduate Level — ***Bryan Goldsmith***
1:30 Paper 506d: Problem-Based Learning on Incorporation of Data Analysis Skills into a Senior Course — ***Helen Lou***, *Yifan Chen, Ravinder Singh*
2:00 Paper 506e: Chemical Engineering Analysis through Systematic Optimization — ***Weiguo Xie***, *Richard A. Davis*
2:30 Paper 506f: Teaching Domain Experts Data Science: A Progress Report from a Purdue Initiative — ***Brett Savoie***

(507) Thermodynamics of Biomolecular Folding and Assembly

Wednesday, Nov 10, 12:30 PM
Marriott Copley Place, Salon C/D

Diwakar Shukla, Chair
Gül Zerze, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

12:30 Paper 507a: The Role of Complementary Shape in Protein Dimerization— ***Fengyi Gao***, *Jens Glaser, Sharon Glotzer*
12:45 Paper 507b: Using a Coarse-Grained Modeling Framework to Identify Oligomeric Motifs with Tunable Secondary Structure — ***Christopher Walker***, *Garrett Meek, Theodore Fobe, Michael Shirts*
1:00 Paper 507c: Exploring Residue Roles in CATCH Peptide Co-Assembly— ***Xin Dong***, *Gregory A. Hudalla, Dillon T. Seroski, Renjie Liu, Carol Hall*
1:15 Paper 507d: Studying Self-Assembly of Key Motifs in N-Terminal of α-Synuclein Using Discontinuous Molecular Dynamics Simulations — ***Van Thanh Tran Nguyen***, *Sabine Ulamec, David Brockwell, Sheena E. Radford, Carol Hall*
1:30 Paper 507e: Inhibition of Amyloid-β Fibril Growth By Enforced Restructuring of the Transition State for Incorporation — ***Sima Mafimoghaddam***, *Yuechuan Xu, Michael Sherman, Prashant Karki, Mehmet Orman, Peter Vekilov*
1:45 Paper 507f: Molecular Simulations to Compute the Dimerization Free Energy of Interferon Regulatory Factor Proteins and Effects of Binding of Ligands on the Dimerization. — ***Ramin Mehrani***, *Sumit Sharma*
2:00 Paper 507g: The Disordered Domain of the Tumor Suppressor p53 Is a Passive Bystander in Mesoscopic Aggregation and Fibrillization. — ***David Yang***, *Weichun Pan, Michael Sherman, Mohammad Safari, Olga Samoylova, Anatoly Kolomeisky, Peter Vekilov*

(508) Value-Added Chemicals from Natural Gas I

Wednesday, Nov 10, 12:30 PM
Marriott Copley Place, Fairfield

Dushyant Shekhawat, Chair
Jared Ciferno, Co-Chair
Goetz Veser, Co-Chair
Jianli Hu, Co-Chair

Sponsored by: Fuels and Petrochemicals Division

12:30 Paper 555a: Chemical Looping for Modular Conversion of Rejected Ethane to Liquid Fuels: Feasibility and Economics — ***Luke Neal***, *Leo Brody, Fanxing Li*
12:50 Paper 555b: Improving Hydrocarbon Yield Via Co-Feeding in Methane Coupling Reaction on Iron/Quartz Catalyst — ***Emily Schulman***, *Su Cheun Oh, Zixiao Liu, Limei Qiu, Yuxia Diao, Guangtong Xu, Asher Leff, Dat T. Tran, Dongxia Liu*
1:10 Paper 508c: Ni/Siralox Catalysts for Ethylene Oligomerization: Effects of Si/Al Ratio on Ni Speciation and Catalytic Performance — ***Joseph McCaig***, *H. Henry Lamb*
1:30 Paper 508d: C123: From Methane to Value-Added C3 Chemicals Via Ethylene — ***Jeroen Poissonnier***, *Alvaro Amieiro Fonseca, Morten Frøseth, Andreas Meiswinkel, Hans-Jörg Zander, Jerome Canivet, Richard Heyn, Joris Thybaut*
1:50 Paper 508e: Towards Elucidating and Accelerating Catalyst Activation in Methane Dehydroaromatization over Fe-ZSM-5 — ***Yifan Deng***, *Goetz Veser*
2:10 Paper 508f: Ethane Dehydroaromatization Using Molybdenum Promoted Microwave Synthesized Zeolites — ***Ashley Caiola***, *Brandon Robinson, Jianli Hu*
2:30 Paper 508g: Feasibility of Chemical Looping Ammonia Synthesis from Metal Nitrides and Hydrides and Their Alloys. — ***Laron Burrows***, *George Bollas*

(509) Poster Session: Catalysis and Reaction Engineering (CRE) Division

Wednesday, Nov 10, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, Exhibit Hall C/D

Shaama Mallikarjun Sharada, Chair
Thomas Schwartz, Co-Chair
Jesse Bond, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

Poster 190e: Origin of Selective Production of Hydrogen Peroxide By Electrochemical Oxygen Reduction — ***Yuanyue Liu***

Poster 717a: Crystalline Mixed Metal Oxides for CO_x-Free Hydrogen Production By Direct Catalytic Decomposition of Methane — ***Hannah Harbin***, *Jordan Chenault, Dominick Casadonte, Sheima Khatib*

Poster 717d: Low Sooting Tendencies and Structure-Property Relationships of Individual Polyoxymethylene Ethers As Alternative Diesel Fuels — ***Junqing Zhu***, *Fan Liang Chan, Thomas D. Foust, Hyunguk Kwon, Stephen Lucas, Lisa D. Pfefferle, Bret C. Windom, Yuan Xuan, Charles S. McEnally*

Poster 509cw: Development of sustainable polyurethanes and polyesters from biomass-derived diols by aldol-condensation and controlled hydrogenation— ***Hochan Chang***, *George Huber, James A. Dumesic*

Poster 509a: Design Rationales for an Optimal Oxide/Metal Interface Catalyst for Hydrodeoxygenation Chemistry of Biomass Derivatives — ***Shyam Deo***, *Kelly Weikel, Michael J. Janik*

Poster 509b: Sustainable Sulfonated Carbons as Esterification Catalysts for the Production of Biochemicals — ***Sarada Sripada***, *James Kastner*

Poster 509c: Identification of Known and Novel Monomers for Poly(hydroxyurethanes) from Biobased Materials — ***Guanhua Wang***, *Linda Broadbelt, Matthew W. Coile, Lauren Lopez, John Torkelson, Yixuan Chen*

Poster 509d: Optimization of Reaction Conditions in the Epoxidation and Hydroxylation of High-Oleic Palm Oil — ***Wilson Felipe Bohorquez Malaver Sr.,Alvaro Orjuela Sr.***, *Paulo Narvaez, Juan Cadavid Sr., Jesus Garcia Sr.*

Poster 509f: Synthesis and Evaluation of Mesoporous Carbons (Starbons®) from Colombian Cassava As Catalyst for Fatty Acids Esterification. — ***Milena Zabala***, *Alvaro Orjuela, Suranjana Bose*

Poster 509j: Modeling Organic Photoredox Catalyst Reduction Kinetics, Donor-Acceptor Interactions, and Degradation Pathways in CO_2 Reduction Catalytic Cycle — ***Kareesa Kron***, *Shaama Mallikarjun Sharada*

Poster 509k: New Horizons for Thermochemical Valorization of CO_2: Efficient Ni@Ni-O-K Catalyst for Low-Temperature Rwgs Reaction — *Lola Azancot, Luis. F Bobadilla, Anna Penkova, Miguel A. Centeno,* ***José A. Odriozola***

Poster 509m: Bioinspired Photocatalytic CO_2 Reduction Exploiting CO_2 Direct Air Capture (DAC) — ***Rito Yanagi***, *Tianshuo Zhao, Matthew Cheng, Shu Hu*

Poster 509o: Kinetic Analysis of 3D-Printed Dual Functional Monoliths in Combined CO_2 Capture-Ethane Dehydrogenation to Ethylene — ***Khaled Baamran***, *Fateme Rezaei, Ali Rownaghi*

Poster 509p: Developing Metal Carbide Nanomaterials for Hydrocarbon and Carbon Dioxide Conversions — ***Junjun Shan***, *Hui Wang, Aihua Zhang, Louis Guillen, Lisa Nguyen, Saydul Sardar, Fu-Kuo Chiang, Jihong Cheng*

Poster 509r: Tungsten Carbides As Active Catalysts for CO_2 Hydrogenation— ***Mitchell B. Juneau***, *Marc Porosoff*

Poster 509s: Enhanced Stability of Fe-Modified CuO-ZnO-ZrO_2-Al_2O_3/HZSM-5 Bifunctional Catalysts for Dimethyl Ether Synthesis Via CO_2 Hydrogenation— ***Xiao Fan***, *Shoujie Ren, Baitang Jin, Shiguang Li, Miao Yu, Xinhua Liang*

Poster 509t: Synthesis of Symmetrical Urea Derivatives from CO_2 and Amines over Copper-Based Core-Shell Catalysts — ***Cihad Karacam***, *James McGregor*

Poster 509u: CO_2 Hydrogenation to Ethanol over Pd/Bi_2O_3 Catalysts: The Synergistic Effect of Pd Particle Size and Surface Oxygen Vacancy — ***Yang Xiao***, *Arvind Varma*

Poster 509v: Molten-Salt Mediated CO_2 Capture and Utilization for Ethane Oxidative Dehydrogenation with Super-Equilibrium CO_2 Conversion — ***Junchen Liu***, *Yunfei Gao, Xijun Wang, Fanxing Li*

Poster 509w: Self-Assembled Monolayers for Electrocatalysis: A Theoretical Study of CO_2 Reduction Reaction to CO over Ag — ***Zhengyang Yang***, *Fanglin Che, Zhiyong Gu*

Poster 509y: Electrochemical Co-Reduction of CO_2 and Nitrates into Urea on Cu-Co Bimetallic Gas Diffusion Electrodes (GDE) — ***Nishithan Balaji Chidambara Kani***, *Aditya Prajapati, Meenesh Singh*

Poster 509z: Combining Metal Sulfides and Organic Cocatalysts to Overcome the Challenges of Electrochemical CO_2 Reduction — ***Foroogh Khezeli***, *Maggie McGovern, Craig Plaisance*

Poster 509aa: Understanding the Interactions between Bubble Dynamics and Electrochemical Energy Losses in Flow Electrolyzers — ***Andrea Angulo Figueira***, *Miguel Modestino*

Poster 509ac: Probing the Dynamic Surface Reconstruction in Non-Stoichiometric Mixed Metal Oxides during Electrochemical Oxygen Evolution— ***John Carl A. Camayang***, *Samji Samira, Jiyun Hong, Adam Hoffman, Simon Bare, Eranda Nikolla*

Poster 509ad: Highly Boosted Reaction Kinetics in Carbon Dioxide Electroreduction By Surface-Introduced Electronegative Dopants — ***Wanzhen Zheng***, ***Yang Hou***

Poster 509ae: Decorating Copper Nanostructures with Atomic Palladium and Silver Species to Regulate Product Selectivity in CO_2 Electroreduction— ***Manjeet Chhetri***, *John Yeager, Case Sandor, Zehua Jin, Ming Yang*

Poster 509af: Electrochemical Charge Transport in Ionic Liquids for CO2 Conversion to Peroxydicarbonate Anion Using Superoxide Ion — ***Ahmed Halilu***, *Mohamed Kheireddine Aroua, Maan Hayyan, Rozita Yusoff, Hanee F. Hizaddin*

Poster 509ai: First-Principles Analysis of Coverage, Ensemble, and Solvation Effects on Selectivity Trends in NO Electroreduction on Pt3Sn Alloys— ***Siddharth Deshpande***, *Jeffrey Greeley*

Poster 509al: Effects of Molecular Properties on Adsorption Energies of Anionic Adsorbates on Platinum — ***Mohammad Hasibul Hasan***, *Ian McCrum*

Poster 509an: First Principles Modeling of FeN_x Clusters and Defects in Aqueous Acidic Media: Tying Structure to Site Stability and Activity for the Oxygen Reduction Reaction — ***Ankita Morankar***, *Siddharth Deshpande, Zhenhua Zeng, Plamen Atanassov, Jeffrey Greeley*

Poster 509ap: Electrocatalytic Reduction of Nitrobenzene By Iron-Salen Ligand Complexes — ***Joshua Miller***, ***Brandon Perdue***, *Andrew Wong, Michael Janik*

Poster 509ar: Surface Proton Dynamics on $BaZrO_3$: Implications for High Temperature Solid Electrolytes in Electrocatalysis — ***Colin Lehman***, *Aleksandra Vojvodic*

Poster 509as: Characterizing Electrochemical Systems By Volterra Kernel Analysis of Response to Small-Amplitude Oscillatory Voltage Inputs — ***Aditya Limaye***, *Adam P. Willard, Karthish Manthiram*

Poster 509at: Designing Electro-Catalysts for the Oxygen Evolution Reaction: A Prisoner of Adsorbate Scaling Relations — ***Abhinav Sankara Raman***, *Colin Lehman, Aleksandra Vojvodic*

Poster 509au: Microwave Enhanced Decomposition of Methane over Iron to Carbon Nanotubes and Hydrogen — ***Troy Christiansen***

Poster 509av: Enhanced Activity and Stability of MgO-Promoted Ni/Al_2O_3Catalyst for Dry Reforming of Methane — ***Baitang Jin***, *Shiguang Li, Xinhua Liang*

Poster 509aw: Site Requirements and Kinetics of Ethane Oxidative Dehydrogenation over Bulk NiO Based Catalysts — ***Xiaohui Zhao***, *Qianyu Ning, Lars Grabow, Jeffrey Rimer, Praveen Bollini*

Poster 509ay: Explaining Size-Dependent Activity Trends and Identifying the Active Facet of Pt and Rh Nanoparticles for Hydrogenation of Phenol — *Isaiah Barth, James Akinola,* ***Jonathan Lee***, *Oliver Gutiérrez-Tinoco, Udishnu Sanyal, Nirala Singh, Bryan Goldsmith*

Poster 509ba: Role of Metal Speciation on Product Selectivity in the Partial Oxidation of Methane over Trimetal Oxo Clusters in Metal-Organic Framework MIL-100 — ***Jacklyn Hall***, *Praveen Bollini*

Poster 509bb: On the Evolution of Ceria Surfaces Towards Catalyzing Non-Oxidative Alkanol Dehydrogenation - a Transient Kinetic Analysis — ***Sadia Afrin***, *Praveen Bollini*

Poster 509bc: Blending Rule for Predicting the Sooting Tendencies of Gasoline Mixtures from the Individual Components — ***Zhanhong Xiang***, *Hyunguk Kwon, Lisa D. Pfefferle, Yuan Xuan, Junqing Zhu, Charles McEnally*

Poster 509bd: Shell Thickness Optimization for Silicalite-1 Encapsulated Ni/Mg Catalysts for Hydrocarbon Reforming: A Modeling Study — ***Brian Gray***, *John Kuhn, Babu Joseph*

Poster 509bg: Molybdenum Oxide Supported Catalysts for Aldol Condensation— *Mathew Rasmussen,* ***Sean Najmi***, *Giada Innocenti, Simon Bare, Andrew Medford, James Medlin, Carsten Sievers*

Poster 509bl: Sustainable Bromine Generation By Electrochemical Halogen Evolution Using Nitrogen-Doped Carbon Nanostructures — *Deeksha Jain,****Dishari Basu***, *Jonathan Hightower, Anne Co, Aravind Asthagiri, Umit S. Ozkan*

Poster 509bm: Tunable Catalytic Performance of Palladium Nanoparticles for H_2O_2 Direct Synthesis Via Surface-Bound Ligands — ***Lucas Freitas De Lima E Freitas***, *Begoña Puértolas, Jing Zhang, Adam Hoffman, Simon Bare, Javier Pérez-Ramírez, James Medlin, Eranda Nikolla*

Poster 509bn: Nanostructured TiO_2 Cavitation Nuclei for Catalytic Degradation of Methylene Blue with Pulsed Ultrasound — *Umesh Jonnalagadda, Xiaoqian Su,* ***James J. Kwan***

Poster 509bo: The Operating Cycle of NO Adsorption and Desorption in Pd-Chabazite for Passive NO_x Adsorbers — ***Marvi Kaushik***, *Gourav Shrivastav, Tuhin Suvra Khan, M. Ali Haider, Divesh Bhatia*

Poster 509br: Au Based Ni and Co Bimetallic Core-Shell Nanocatalysts for Room Temperature Selective Decomposition of Hydrous Hydrazine to Hydrogen— ***Dr. PREETI Jain***

Poster 509bs: Investigation of Synergistic Interfaces in Metal-Metal Oxide Inverted Systems for Catalytic Upgrading — ***Laura Paz Herrera***, *Lucas Freitas De Lima E Freitas, Eranda Nikolla, James Medlin*

Poster 509bt: Quantifying the Effect of Surface Density of Aminosilanes on the Fraction of Active Sites in SBA-15 for the Aldol Condensation — ***Jee-Yee Chen***, *Nicholas Brunelli*

Poster 509bu: Design and Characterization of Washcoated Catalytic Microreactors for Dynamic Operation — ***Cameron Armstrong***, *Andrew R Teixeira*

Poster 509bw: Supercritical Fluids As Reaction Media for Scalable Production of Carbon Nanomaterials and Their Applications — ***Haider Almkhelfe***

Poster 509bx: Magnesium- PAP Metal Organic Framework Based Photoswitcher for the Degradation of Chlorpyrifos — ***Anita Yadav***, *Anu Sharma, Rakesh Kumar Sharma, Surender Kumar Sharma*

Poster 509by: Molten Salt Synthesis of (Ni,Mg)O Mixed Oxides: Designing New Methods to Control Crystal Morphology — ***Mariano D. Susman***, *Hien N. Pham, Xiaohui Zhao, Raffaele Cheula, David West, Sivadinarayana Chinta, Matteo Maestri, Praveen Bollini, Abhaya K. Datye, Jeffrey Rimer*

Poster 509bz: Understanding Pd-MO Interfaces in Inverted Catalytic Structures— ***Lucas Freitas De Lima E Freitas***, *Laura Paz Herrera, James Medlin, Eranda Nikolla*

Poster 509ca: Influencing Selectivity of Ni Reverse Water Gas Shift Catalysts Using Atomic Layer Deposition — ***Megan English***, *Kent J. Warren, Alan Weimer*

Poster 509cc: Mesoporous Iron Gallate Nanocomplex for Adsorption and Degradation of Organic Dyes — ***Anita Yadav***, *Anu Sharma, Rakesh Kumar Sharma*

Poster 509cf: Development of Methods for Consistently Tuning Silica-Encapsulated Gold Core-Shell Nanoparticle Morphology — ***Ellis Hammond-Pereira***, *Steven Saunders*

Poster 509ci: Autothermal Reactor Design and Development for the Oxidative Dehydrogenation of Ethane — ***Jiakang Chen***, *Praveen Bollini, Vemuri Balakotaiah*

Poster 509cj: Effect of Reactant Identity and Acid-Site Strength on Acid-Catalyzed Aldol Reactions — ***Shubham Malviya***, *Friederike Jentoft, Peng Bai*

Poster 509cl: Tuning the Activity of Benzyl Alcohol Hydrodeoxygenation Using Organic Ligands — ***Zachary Blanchette***, *Daniel K. Schwartz, James Medlin*

Poster 509cn: Integrating Nanostraws in Porous Catalyst Supports to Enhance Molecular Transport to Catalytic Sites — ***Oluwole Ajumobi***, *Yang Su, Azeem Farinmade, Lei Yu, Jibao He, Julia A. Valla, Vijay T. John*

Poster 509co: Effect of Water on Cumene Dealkylation over ZSM-5 Zeolites— ***Han Chau***, *Abhishek Gumidyala, Steven Crossley*

Poster 509cp: First-Principles Calculations to Data-Driven Discovery and Materials Design of Mxene Electrocatalysts — ***Luke Johnson***, ***Brandon Burghardt***, ***Yamilée Morency***, *Aleksandra Vojvodic*

Poster 509cq: Rational Catalyst Design through Computational Catalysis — ***G. T. Kasun Kalhara Gunasooriya***

Poster 509cr: Neural Networks Learn Fundamental Adsorption Energy Scaling Relations — ***Brook Wander***, *Zachary Ulissi*

Poster 509cs: Combining Uncertainty Metrics to Control Neural Network Error and Accelerate Chemical Exploration — ***Eric Musa***, ***Cameron Gruich***, *Frank Doherty, Bryan Goldsmith*

Poster 509ct: An Automated Workflow to Rapidly and Accurately Generate Transition State Structures Using Machine Learning — ***Lagnajit Pattanaik***, *Xiaorui Dong, Kevin Spiekermann, William Green*

Poster 509cv: Catalytic Resonance Theory: Negatively Correlated Linear Scaling Relationships for Overcoming the Sabatier Limit — ***Sallye Gathmann***, *M. Alexander Ardagh, Paul J. Dauenhauer*

Poster 509cw: Accelerating Ammonia Electrooxidation Catalyst Discovery through Interpretable Machine Learning — ***Hemanth Pillai***, *Shih-Han Wang, Luke E. K. Achenie, Hongliang Xin*

Poster 509cx: Grand Canonical Monte Carlo Simulation Methods for Understanding Coke-Resistance Under Dehydrogenation Conditions — ***Peng Wang***, *Thomas Senftle*

Poster 509cy: Chemically-Informed Data-Driven Optimization (ChIDDO): Leveraging Physical Models and Bayesian Learning to Accelerate Chemical Research — ***Daniel Frey***, *Xinshu Shang, Ju hee Shin, Miguel Modestino*

Poster 509cz: Deconvoluting XPS Spectra in Lanthanum-Based Perovskites: An Analysis from First Principles — ***Ariel Whitten***, *Elif Tezel, Dezhou Guo, Mahdokht Soltani, Reinhard Denecke, Eranda Nikolla, Jean-Sabin McEwen*

Poster 509da: Nuclearity As a Descriptor for Site and Surface Selection— ***Unnatti Sharma***, *Zachary Ulissi, Angela Nguyen, Michael J. Janik*

Poster 509db: Developing Linear Free Energy Relationships for Transition Metal Chemistry — ***Zhenzhuo Lan***, *Shaama Mallikarjun Sharada*

Poster 509dc: High Throughput Surface Stability Analysis of Alloy Catalysts Using Density Functional Theory and Machine Learning — ***Gaurav Deshmukh***, *Pushkar Ghanekar, Jeffrey Greeley*

Poster 509de: High Throughput Screening of Bio-Inspired Mo/W Catalysts— ***Mingjie Liu***, *Azadeh Nazemi, Heather Kulik*

Poster 509df: Graph Neural Networks to Predict Thermochemistry of Halogenated Hydrocarbons for Use in Combustion Modeling: New Data, Methods, and a Cautionary Tale. — *Sai Krishna Sirumalla,* ***David Farina Jr.***, *Richard H. West*

Poster 509dg: Computer-Aided Prediction of Enzymatic Reactions — ***Esther Heid***, *Samuel Goldman, Karthik Sankaranarayanan, Connor Coley, Klavs F. Jensen, Christoph Flamm, William Green*

Poster 509dh: Predicting Segregation Energy in Single Atom Alloys Using Physics and Machine Learning — ***Maya Salem***, *Michael Cowan, Giannis Mpourmpakis*

Poster 509dj: Interpreting the Optical Absorption Spectra of Gold Nanoclusters By Convolutional Neural Network — ***Jiali Li***, *Tiankai Chen, Pengfei Cai, Zekun Ren, Yixin Zhu, Jianping Xie, Xiaonan Wang*

Poster 509dl: Fundamental Study of the Relationship between Catalytic Performance and Pretreatment for NO Reduction By CO Reaction over CeO_2supported NiO_x Catalyst — ***Kyung-Min Lee***, *Taejin Kim, Gihan Kwon*

Poster 509dm: Rapid Fabrication of Atomically Dispersed Fe on Porous Carbon Via Photothermal Process for Nitrogen Reduction — ***Hsin-Jung Yu***

(510) Poster Session: Environmental Division

Wednesday, Nov 10, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, Exhibit Hall C/D

Gerardo Ruiz-Mercado, Chair
Kristina Wagstrom, Co-Chair

Sponsored by: Environmental Division

Poster 510a: Continuous Flow Catalytic Hydrogenation of Groundwater Nitrate Using Hydrogen-Permeable Hollow Fiber Membranes Decorated with Palladium-Indium Nanoparticles — ***Juliana Levi***, *Sujin Guo, Juan Donoso, Yihao Luo, Chung-Seop Lee, Chen Zhou, Sergi Garcia-Segura, Michael S. Wong, Bruce Rittmann, Paul Westerhoff*

Poster 510b: Naa Zeolite-Coated Meshes with Tunable Hydrophilicity for Oil-Water Separation — ***Diako Mahmodi***, *Shailesh Dangwal, Seokjhin Kim*

Poster 510c: Cobalt-Based ZIF Coordinated Hybrids with Defective TiO2-x Forboosting Visible Light-Driven Photo-Fenton-like Degradation of Bisphenol a— ***Xiaohong Yin***

Poster 510d: Photocatalytic Removal of Waterborne Pollutants By Electrospun Nanofibers of Graphitic Carbon Nitride and Titanium Nitride — ***Jake Leplatt***,***Zackary Smith***, *Dipendu Saha*

Poster 510f: Synthesis of Imidazole and Amine Based Deep Eutectic Solvents for Low Concentration so_2 Capture — ***Dongwook Lee***, *Cristian Aravena, Won Yong Choi, Kyumin Jang, Injun Kim, Yunsung Yoo, Jinwon Park*

Poster 510g: Finding Properties Effecting Selectivity of SeO_4^{2-} Removal from Water Containing Se/S/P Oxo-Anions Using Adsorption on Metal Oxide: DFT Study with Hybrid Solvent Method. — ***Srishti Gupta***, *Anh Nguyen, Christopher L. Muhich*

Poster 510h: A Comparative Study of the Thermal and Hydrothermal Aging Effect on Cu-SSZ-13 for the Selective Catalytic Reduction of NOx with NH_3— ***Huawang Zhao***

Poster 510i: Characterization of Lethal Toxicity of Engineered Nanoparticles on Isochrysis Galbana Via Guts-Derived Fate-Transport-Effect Model — ***Joshua Prince***, *A-Andrew D. Jones III*

Poster 510j: Techno-Economic Analysis and Life Cycle Assessment of Contaminant Removal from Landfill Gas for Electricity Generation. — ***Rarosue Amaraibi***, *Babu Joseph, John Kuhn*

Poster 510n: Leaching and Fixation of Heavy Metals in Municipal Solid Waste Incineration Fly Ash (MSWI FA) Based on CO_2 Uptake Process — ***Dongwoo Kang***, *Yunsung Yoo, Jinwon Park*

Poster 510q: Life Cycle Comparison of Battery Recycling and Raw Material Extraction — ***Samantha Bunke***, *Xi Chen, Michael Machala, Ines Azevedo, Sally Benson, William Tarpeh*

Poster 510r: Modeling Bioplastic Production from Astronaut Organic Wastes for Resource Recovery Using Coupled Anaerobic-Aerobic Bioreactors for Long-Duration Space Operations — ***Thomas Rafferty***, *MacKenzie Burns, Ian Morris, Marley Wait, Emma Begin, Kourtney Zeiler, Chelsea Q Linvill, Michael Butkus, Corey James, Andrew Pfluger*

Poster 510s: Optimizing Chemical Recycling of Waste PET/Polyolefin Streams through Agile Life Cycle Assessment (LCA) — ***Md Nurus Sakib***, *Rui Shi*

Poster 510t: Evaluation of *Galdieria Sulphuraria* for the Bioremediation of Produced Water — ***Ashiqur Rahman***, *Shanglei Pan, Cymone Houston, Tracy Benson, Thinesh Selvaratnam*

(511) Poster Session: Particle Technology Forum

Wednesday, Nov 10, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, Exhibit Hall C/D

Michael Molnar, Chair

Sponsored by: Particle Technology Forum

Poster 511c: A Moving Porous Media Model for Simulations of Continuous Spatial Particle ALD — ***Julia Hartig***, *Davis R. Conklin, Alan Weimer*

Poster 511d: *What Is More Important for Improved Drug Dissolution: Agglomerate Size Reduction or Enhancing Particle Surface Wettability?*— ***Sangah Kim***, *Hira Khurshid, Rajesh Dave*

Poster 511g: Radiation Heat Transfer in a Rotary Drum — ***Bhaumik Bheda***, *Heather Emady*

Poster 511i: Effect of Dopant Modification in Iron Sulfide-Based Sulfur Carrier for Hydrogen Production from Hydrogen Sulfide in a One-Reactor Cyclic Sulfur Looping Scheme — ***Kalyani Jangam***, *Yu-Yen Chen, Lang Qin, L.-S. Fan*

Poster 511j: Mastering the Processing Methods of Engineered Particles— ***Willie Hendrickson***, *Chris Rueb, Charles Bowman, Robert G. Bowman*

Poster 511l: Microstructure Design and Release Kinetics of Layer-Wise Agglomerated Granules — ***Camila Garcia Jange***, *Carl R. Wassgren, Kingsly Ambrose*

Poster 511m: Analysis of Structure Formation and Layer Build-up from Dried Deposited Nanoparticle Suspension Droplets — ***Manuel Janocha***, *Evangelos Tsotsas*

(512) Poster Session: Process Development

Wednesday, Nov 10, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, Exhibit Hall C/D

Deepak Sharma, Chair
Vinod Kumar Venkatakrishnan, Co-Chair

Sponsored by: Process Development Division

Poster 512a: Efficient Process for the Production of High Conductivity, Carbon-Rich Materials from Coal — ***Min Song***, *Jake Herb, David Gamliel, Nathan Shipley, Gabrielle Aversa, Caitlin Bien, Christopher Lang, Zachary Whitermore, Jeffrey Yee, Dorin Preda*

Poster 512b: Modular Processing of Flare Gas for Hydrogen and Carbon Nanofibers — ***Jessica Hauck***, *Kent J. Warren, Gage Sowell, Theodore Champ, Mija H. Hubler, Linfei Li, Boning Wang, Robert L. Anderson, Andrew Broerman, Alan Weimer*

Poster 512e: Modeling Particle Atomic Layer Deposition in a Fluidized Bed with CFD-DEM — ***Davis Conklin***, *Julia Hartig, Alan Weimer*

Poster 512f: Study and modeling the wettability contact angle and area measurement for EOR in 2D imaging technology by using python algorithm— ***Hussain Alajaj***, *Ralph E. Flori Jr., Waleed Al-Bazzaz*

(513) Poster Session: Sustainability and Sustainable Biorefineries

Wednesday, Nov 10, 3:30 PM

John B. Hynes Veterans Memorial Convention Center, Exhibit Hall C/D

Clayton Jeffryes, Chair
Julia Lin, Co-Chair
Ashley Pennington, Co-Chair

Sponsored by: Sustainable Biorefineries

Poster 509bk: Upcycling Plastic Waste into Plastic Derived Cooking Fuel in Developing Countries — ***Shelby Browning***, *Jeffrey Seay, Betsy Beymer-Farris*
Poster 374f: A Comparison of Solar Methanol and Ammonia Production Explicitly Accounting for Intermittency — ***Caroline Ganzer***, *Niall Mac Dowell*
Poster 566e: Decarbonisation of Power and Industry in the UK — ***Caroline Ganzer***, *Niall Mac Dowell*
Poster 513b: Remediating Corn Ethanol Waste Stillage with *Chlorella vulgaris*— ***Ankit Nayar***, *Kelvin Elgar, Prasad Pawar, Melody Youwakim, Clayton Jeffryes*
Poster 513c: A Community-Level Energy Planning Model for the Dynamic Optimization of Waste-to-Gas and Waste-to-Power Anaerobic Digestion Supply Chains — ***Irene Mas Martin***, *Alvina Aui, Lisa Schulte, Mark Mba Wright*
Poster 513e: CO_2 Capture Using Amine-Functionalized Fumed Silica Via Molecular Layer Deposition — ***Hailey Loehde-Woolard***, *Annika Lai, William McNeary IV, Jessica Burger, Robert Pfeffer, Alan Weimer*
Poster 513f: Lignin-First Strategy for Upgrading Lignin into Value-Added Products: Maximizing Feedstock Utilization — ***Canan Sener***, *Miguel Perez, German Umana, Shamik Misra, Christos Maravelias, Steven D. Karlen, Timothy J. Donohue, Daniel R. Noguera, John Ralph*
Poster 513g: Water Retention Value As a Characterization Approach for Predictive Modeling of Corn Stover Deconstruction — ***William Otto***, *Dylan Cousins, David Hodge*
Poster 513h: Pretreatment of Used Cooking Oils and Recovery of Free Fatty Acids Via Liquid-Liquid Extraction in a Falling Film Contactor — ***Juliana Cardenas***, *Alvaro Orjuela, Paulo Narvaez, Benjamin Katryniok, James Clark*
Poster 513j: The Hybrid Kinetic-Optimization Modeling and Machine-Learning (ANN and SVM) of Biomass (Maple Leaf) Pyrolysis — ***Hui Liu***, *Muhammad Ahmad, Hesham Alhumade, Shivkumar Bale, Ali Elkamel*
Poster 513k: Experimental and Theoretical Studies of an Iron-Based Oxygen Carrier with a Core-Shell Structure of Fe_2O_3@CeO_2 for Chemical Looping Biomass Gasification — ***Afsaneh Khajeh***, *Hessamedin Naeimi, Lijun Wang, Abloghasem Shahbazi*
Poster 513l: One-Step Catalytic Fast Hydropyrolysis and Upgrading of Biomass to Biofuels Using MCM-41/ZSM-5 Composites — ***Lei Yu***, *Azeem Farinmade, Oluwole Ajumobi, Vijay T. John, Julia A. Valla*
Poster 513m: CFD Model Investigation of Syngas Production Process through Chemical Looping Gasification of Biomass in Fluidized Bed Reactor— ***Hessamedin Naeimi***, *Afsaneh Khajeh, Lijun Wang, Abloghasem Shahbazi*

(514) Advanced Organic/Inorganic Materials for Membrane Gas Separation

Wednesday, Nov 10, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 300

Seokjhin Kim, Co-Chair
Piran Kidambi, Co-Chair

Sponsored by: Membrane-Based Separations

3:30 Paper 514a: Fabrication of Silicon-Based Ceramic Membranes Via Pyrolysis of Plasma Deposited Polymer Films — ***Bryan Nguyen***, *Nicholas Welchert, Malancha Gupta, Theodore T. Tsotsis*
3:45 Paper 514d: Immobilized Molten Salt Membranes for Ammonia Purification— ***Rok Sitar***, *Zhenyu Zhang, Javishk Shah, Jolie Lucero, Hope Wikoff, J. Douglas Way, Colin A. Wolden*
4:00 Paper 514f: Facilitated Transport Membranes for H_2 Purification from Coal-Derived Syngas: A Techno-Economic Analysis — ***Yang Han***, *W.S. Winston Ho*
4:15 Paper 514g: Polybenzimidazole-Derived Asymmetric Carbon Molecular Sieve Hollow Fiber Membranes for Gas Separations — ***Jong Geun Seong***, *Jeremy Lewis, John Matteson, Harshul Thakkar, Erica Craddock, Kathryn A. Berchtold, Rajinder P. Singh*

(515) Analysis and Assessment for Solving the Plastic Waste Crisis

Wednesday, Nov 10, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 200

Steve Duke, Co-Chair
Jeffrey Seay, Co-Chair

Sponsored by: Waste Plastics

3:30 Paper 515a: Wolfsat-1: A Cubesat Mission to Investigate the Metabolism in Microgravity of the Polyethylene Digesting *Ideonella Sakaiensis*. — ***Mili Mohanty***, ***Michael Mikati***, ***Paul Kiesling***, ***Kevin Simmons***
3:51 Paper 515b: Rapid and Real-Time Mixed-Plastic Waste Analysis Using Infrared Spectroscopy and Machine Learning — ***Shengli Jiang***, *Victor M. Zavala*
4:12 Paper 515c: Efficient Biodegradation of Poly(ethylene Terephthalate) with Leaf-Branch Compost Cutinase — ***Ya-Hue Soong***, *Akanksha Patel, Na Liu, Hsi-Wu Wong, Margaret J. Sobkowicz, Dongming Xie*
4:33: Break
4:54 Paper 515f: An Assessment of Methodologies Offered for Valuable Metal Recovery from E-Waste Scraps — ***Aman Singh***, *Dr. Utkarsh Maheshwari*
5:15 Paper 515g: The Use of Life Cycle Assessment to Identify Sustainability Characteristics of Plastic Recycling Systems: A Review — ***Md Nurus Sakib***, *Rui Shi*

(516) Applied Math for Biological and Biomedical Systems

Wednesday, Nov 10, 3:30 PM
Sheraton Back Bay, Independence Ballroom East

Ashlee Ford Versypt, Chair
Dongheon Lee, Co-Chair

Sponsored by: Applied Mathematics and Numerical Analysis

3:30 Paper 516a: Semi-Structured Kinetic Modeling of a Methanotroph-Cyanobacteria Coculture Can Quantify the Effect of Unknown Metabolic Interactions on Enhancing Coculture Growth — ***Kiumars Badr***, *Q. Peter He, Jin Wang*
3:49 Paper 516b: Unveiling Metabolic Requirements for Gluconeogenesis through Kinetic Modeling and Optimization — ***Yen-An Lu***, *Conor O'Brien, Wei-Shou Hu, Qi Zhang*
4:08 Paper 516c: Predicting Colorectal Cancer from Human Gut Microbiome Data — *Mitchell Daneker,* ***Linh Nguyen***, *Ryan Terrel, Babatunde A. Ogunnaike, Prasad Dhurjati*
4:27 Paper 516d: Extensional Stresses on Vwf Proteins in Turbulent Flows— ***Oanh Pham***, *Samuel E. Feher, Quoc T. Nguyen, Dimitrios Papavassiliou*
4:46 Paper 516e: Predict the Effect of Disease-Specific Airway Deformation Kinematics on Dry Powder Transport and Deposition in Whole Lung — *Jianan Zhao,* ***Yu Feng***, *Ahmadreza Haghnegahdar, Rahul Bharadwaj*
5:05 Paper 516f: Up, up, and Away: A Physiologically-Motivated Dynamic Model of the Lung's Mucociliary Clearance Escalator — ***Monica Shapiro***, *Timothy Corcoran, Carol A. Bertrand, Robert Parker*
5:24 Paper 516g: Collagen Deposition during Diabetic Kidney Disease Enhances Cellular Communication — ***Haryana Thomas***, *Ashlee Ford Versypt*
5:43 Paper 516h: Smart Perfusion Machines — *Emily Ferrarese,* ***Angelo Lucia***, *Korkut Uygun*

(517) Area Plenary: Electronic and Photonic Materials - Industry and Academia (Invited Talks)

Wednesday, Nov 10, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 103

Charles Hages, Chair

Sponsored by: Electronics and Photonics

3:30 Paper 517a: Electronic Materials for a New Era of Computing — ***Kevin Brew***
3:55 Paper 517e: Materials and Challenges for Deep UV Emitters — ***Eric Bretschneider***
4:20 Paper 517b: New plasma physics and materials to unlock economic use of terrestrial thermionic converters — ***Max Mankin***
4:45 Paper 517d: Quantifying Carrier Recombination to Accelerate Development of High-Efficiency Solar Cells — ***Jason Baxter***
5:10 Paper 517c: Commercializing Perovskite Tandem Solar Cells — ***Rohit Prasanna***

(518) Biochemical Conversion Processes in Forest/Plant Biomass Biorefineries

Wednesday, Nov 10, 3:30 PM
Marriott Copley Place, Exeter

Shijie Liu, Chair

Sponsored by: Forest and Plant Bioproducts Division

3:30: Break
3:45: Break
4:00: Break
4:15 Paper 518d: Modeling Heat Transfer and Reaction Kinetics of Biomass in Pyrolysis Feeding Systems — ***Jessie Troxler***, *Tim Dunning, Jonathan Stickel, Joseph Samaniuk, Daniel Carpenter*
4:30 Paper 518e: High Yield Synthesis of HMF from Glucose in the Water-Organic Solvent System — ***Ravikumar Gogar***, *Sridhar Viamajala, Patricia Relue, Sasidhar Varanasi*

(519) Biomass Characterization, Pretreatment, and Fractionation

Wednesday, Nov 10, 3:30 PM
Marriott Copley Place, Provincetown

Catherine Brewer, Chair

Sponsored by: Forest and Plant Bioproducts Division

3:30 Paper 519a: Characterization of Transgenic Sugarcane (lipidcane 1566) and Its Potential As a Raw Material for Co-Production of Ethanol and Biodiesel— ***Mothi Bharath Viswanathan***, *Shraddha Maitra, Kiyoul Park, Edgar Cahoon, Fredy Altpeter, Andrew D. B. Leakey, Scott McCoy, Vijay Singh*
3:45 Paper 519b: Hot-Water Pretreatment and Saccharification of Genetically Modified Cellulosic Feedstock for Fuel Production — ***Ramkrishna Singh***
4:00 Paper 519c: Coupled Near Infrared Spectroscopy and Air Classification of Corn Stover for Improved Feedstock Quality — ***Dylan Cousins***, *Jeffrey A. Lacey, John E. Aston, David Hodge*
4:15 Paper 519d: Lignin Extraction from Cellulose in Loblolly Pine Using Deep Eutectic Solvent Screening with COSMO — ***Thomas Quaid***, *Toufiq Reza*
4:30 Paper 519e: One-Step Extraction of Multifunctionalized Lignins from Biomass — ***Stefania Bertella***, *Jeremy Luterbacher*
4:45 Paper 519f: Deashing of Biomass By Deep Eutectic Solvent to Enhance Biomass Conversion Process — ***Md Tahmid Islam***, *Jordan Klinger, Toufiq Reza*
5:00 Paper 519g: Lignin-Based Deep Eutectic Solvent Pretreatment of Transgenic Sweet Sorghum Bagasse to Achieve a Sustainable Biorefinery Process — ***Yunxuan Wang***, *Xianzhi Meng, Yang Tian, Linjing Jia, Aymerick Eudes, Kwang Ho Kim, Yunqiao Pu, Gyu Leem, Deepak Kumar, Arthur J. Ragauskas, Chang Geun Yoo*

5:15 Paper 519h: Resolving the Discrepancies in the True Molecular Weight of Lignins with the Assistance of the ALPHA Process — ***Zachariah Pittman***, *Graham Tindall, Mark Thies, Christopher Kitchens*

(520) Biomaterials I

Wednesday, Nov 10, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 104

Jorge Almodovar, Chair
Kelly Burke, Co-Chair
Kyung-Ho Roh, Co-Chair
Shreyas Rao, Co-Chair

Sponsored by: Biomaterials

3:30 Paper 520a: Bio/Nanomaterials for Control of Stem Cell Fates and for Biomolecule Delivery — ***Surya Mallapragada***
4:06 Paper 520b: Surface Modification with Heparin-Collagen Layer-By-Layer Coatings Enhances Adherence, Cell Migration, and Protein Expression in Human Schwann Cells — ***Luis Carlos Pinzon-Herrera***, *Jorge Almodovar*
4:24 Paper 520c: 3D Bioprinting of Hydrogel Constructs for Integration with Islet Organ-on-Chip System — ***Miranda Poklar***, *Ravi Krishnamurthy, Connor Wiegand, Prashant Kumta, Ipsita Banerjee*
4:42 Paper 520d: Mechanical Evaluation of Silk Fibroin Collected from Plodia Interpunctella: An Alternative Source of Silk for Biomedical Applications — *Bryce Shirk, Ali Lateef, Paul Shirk,* ***Whitney Stoppel***
5:00 Paper 520e: Direct Contact with Astrocytes Drives Metabolic Reprogramming in Glioblastoma Multiforme Cells — ***Kimberly M Stanke***, *Christina Wilson, Oleh Khalimonchuk, Srivatsan Kidambi*
5:18 Paper 520f: Stiffening Hydrogels to Study Human Lung Fibroblast Activation and Mechanical Memory — ***Jenna Sumey***, *Steven Caliari*
5:36 Paper 520g: Engineering DNA-Based and Protein-Based Materials for Live Single Cell Analysis — ***Sasha Ebrahimi***, *Chad A. Mirkin*

(521) Bionanotechnology Graduate Student Award Session II

Wednesday, Nov 10, 3:30 PM
Marriott Copley Place, Simmons

Catherine Fromen, Chair
Lorraine Leon, Co-Chair
Elizabeth Nance, Co-Chair

Sponsored by: Bionanotechnology

3:30 Paper 521a: Award Submission DNA Origami Tubes with Reconfigurable Cross-Sections — ***Anjelica Kucinic***, *Chao-min Huang, Jingyuan Wang, Carlos E. Castro*
3:50 Paper 521b: Nanoconfined Water Endows Peptidoglycan Extreme Water-Responsive Actuation — ***Zhi-Lun Liu***, *Haozhen Wang, Xi Chen*
4:10 Paper 521c: Polypeptide Templating of Structural Proteins for Tailored Hierarchical Materials — ***Hui Sun***, *Benedetto Marelli*
4:30 Paper 521d: Synthesis and Characterization of Biogenic Selenium Nanoparticles Made from Pathogenic Bacteria with Selective Antimicrobial Properties — ***Linh Truong***, *David Medina, Thomas J. Webster*
4:50 Paper 521e: Single Particle ICP-MS: An Emerging Technique for Quantifying Size and Aggregation of Inorganic Nanomaterials for Biomedical Applications — ***Nathan Donahue***, *Emmy Francek, Emi Kiyotake, Emily Thomas, Wen Yang, Lin Wang, Michael Detamore, Stefan Wilhelm*
5:10 Paper 521f: Multispectral Fingerprinting Resolves Dynamics of Nanomaterial Trafficking in Primary Endothelial Cells (Award Session)— ***Mitchell Gravely***, *Daniel Roxbury*

(522) Characterization of Non-Newtonian Fluids

Wednesday, Nov 10, 3:30 PM
Sheraton Back Bay, Constitution B

Jeffrey J. Richards, Chair
Qin Qi, Co-Chair

Sponsored by: Fluid Mechanics

3:30 Paper 522a: Non-Viscometric Flow of Yield Stress Fluids: Flow Visualization, Velocimetry and Finite Element Modeling — *Anthony McMaster, Josh McConnell,* ***Anne M. Grillet***, *Christine Cardinal Roberts, Jonathan Leonard, Simon Rogers, Rekha R. Rao*
3:45 Paper 522b: Going with the Flow: Colloidal Dynamics at Moving Immiscible Fluid Interfaces — ***Joanna Schneider***, *Rodney Priestley, Sujit Datta*
4:00 Paper 522c: Non-Newtonian Neural Network, N^4, a Machine Learning Framework for Solving Non-Newtonian Fluid Problems — ***Mohammadamin Mahmoudabadbozchelou***, *George Em Karniadakis, Safa Jamali*
4:15 Paper 522d: The Influence of Surface Properties and Interfacially-Active Species on the Coalescence-Mediated Wetting of a Surface By an Emulsion Drop — *Suraj Borkar,* ***Arun Ramchandran***
4:30 Paper 522e: A General Solution for Equations of Poroelasticity — ***Moslem Moradi***, *Ehssan Nazockdast*
4:45 Paper 522f: Quincke Oscillations of Colloids at Planar Electrodes — *Zhengyan Zhang, Hang Yuan, Yong Dou, Monica Olvera De La Cruz,* ***Kyle Bishop***
5:00 Paper 522g: Nuclear Magnetic Resonance Diffusometry of Linear and Branched Worm-like Micelles — *Samuel W. Holder, Samuel C. Grant,* ***Hadi Mohammadigoushki***
5:15 Paper 522h: Depletion and Electrostatic Forces in Shear Rheology of Cellulose Nanofiber Suspensions — ***Behzad Nazari***, *Douglas Bousfield*
5:30 Paper 522i: In-Situ Microrheology of Drying Paint — ***Maria Chiara Roffin***, *Christopher Wirth, Steven Barancyk, Reza Rock, Andy Surface, James Gilchrist*
5:45 Paper 522j: Life Expectancy and Mileage of Colloidal Bonds in Attractive Colloidal Gels — ***Safa Jamali***, *Safa Jamali*

(523) Charged and Ion-Containing Polymers: Polyelectrolyte Solutions and Complex Coacervates

Wednesday, Nov 10, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 105

Samanvaya Srivastava, Chair
Xiaoxue Wang, Co-Chair
Whitney Loo, Co-Chair
Hee Jeung Oh, Co-Chair

Sponsored by: Polymers

3:30 Paper 523a: A High-Throughput Study of Polyelectrolyte Complex Coacervate Rheology and Structures — ***Yimin Luo***, *Chelsea Edwards, Mengyang Gu, Yue He, Megan T. Valentine, Matthew Helgeson*
3:45 Paper 523b: Reproducible Measurements of Linear Viscoelasticity of Polyelectrolyte Coacervates in the Low-Frequency Region, Including Emergence of a Low-Frequency Plateau — ***Huiling Li***, *Ying Liu, Erdem Ozdemir, Ronald Larson*
4:00 Paper 523c: pH Effects in Polymeric Complex Coacervation — *Ashley R. Knoerdel, Whitney C. Blocher McTigue,* ***Charles Sing***
4:15 Paper 523e: Predicting Polyelectrolyte Complex Coacervation from a Molecularly-Informed Field-Theoretic Simulation Approach — ***My Nguyen***, *Nick Sherck, Kevin Shen, Brian Yoo, Stephan Kohler, Joshua Speros, Kris Delaney, M. Scott Shell, Glenn H. Fredrickson*
4:30 Paper 356l: Scaling Theory of Single-Chain Sequence-Specific Polyampholytes — ***Artem Rumyantsev***, *Nicholas Jackson, Albert Johner, Juan J. de Pablo*
4:45 Paper 523h: Vesicle-Stabilized Polyelectrolyte Complex Coacervate Emulsions — ***Shang Gao***, *Samanvaya Srivastava*
5:00 Paper 523i: Interfacial Crosslinking of Polyelectrolyte Complex Coacervate Droplets in Non-Equilibrium Supernatant — ***Aman Agrawal***, *Jack F. Douglas, Alamgir Karim*
5:15 Paper 523j: Exploring the Effects of Osmolytes on Complex Coacervation— ***Xianci Zeng***, *Alex Lawton, Pratik Joshi, Caryn Heldt, Sarah L. Perry*
5:30 Paper 523d: Effect of Salt Addition on the Phase Behavior and Rheological Properties of Natural Polyelectrolyte Complexes — ***Anandavalli Varadarajan***, *Santanu Kundu*
5:45 Paper 733d: Polyelectrolyte Complex Coacervation across a Broad Range of Linear Charge Densities — ***Angelika Neitzel***, *Yan Fang, Boyuan Yu, Artem Rumyantsev, Juan J. de Pablo, Matthew V. Tirrell*

(524) Computational Solid State Pharmaceutics

Wednesday, Nov 10, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 102

Yuriy Abramov, Co-Chair
Ebenezer Ojo, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

3:30 Paper 524c: Optimizing Sampling Efficiency in the Einstein Crystal Free Energy Method — ***Eric Dybeck***
3:54 Paper 524d: Physics-Based Computational Models to Expedite Pharmaceutical Solid-Form Selection — *Chandler Greenwell, Qun Zeng, Chao Chang, Zhuocen Yang, Yuriy Abramov, Shanming Kuang, San Kiang, Jian Wang, Sivakumar Sekharan*
4:18 Paper 524e: Morphology Prediction for Crystals Using Hybrid Force Field— ***Yongsheng Zhao***, *Michael F. Doherty*
4:42 Paper 308c: Development of RTD-Based Flowsheet Modeling Including Process Uncertainty for Continuous Solid-Based Drug Manufacturing — ***Huayu Tian***, *Pooja Bhalode, Sonia M. Razavi, Andres Roman-Ospino, Fernando Muzzio, Marianthi Ierapetritou*
5:06 Paper 524f: Computational Fluid Dynamics Study to Resolve Mixing and Scale-up Challenges of Non-Newtonian Fluids in Pharmaceutical Industry— ***Nikhil Srivastava***, *Saurav S. Rath, SVB Janardhan Garikipati, Birendra K. David*

(525) Computational Studies of Early-Stage and Low-Dimensional Self-Assembly

Wednesday, Nov 10, 3:30 PM
Marriott Copley Place, Salon H/I

Julia Dshemuchadse, Chair
Sumit Sharma, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

3:30 Paper 525a: Mesoscale Simulation Approach for Dynamics and Assembly of Deformable Objects — ***Patrick Underhill***
3:45 Paper 525b: Entropy Compartmentalization of Open Host-Guest Colloidal Clathrates with Rotating Guest Particles — ***Sangmin Lee***, *Sharon Glotzer*
4:00 Paper 525c: Effect of Particle Anisotropy and Rotational Symmetry on the Kinetics of Disorder-to-Order Phase Transitions — ***Abhishek Sharma***, *Fernando Escobedo*
4:15 Paper 525d: Two-Dimensional Self-Assembly of "Ionic" Colloidal Crystals— ***Jasmin J. Kennard***, *Caleb D. Biddulph, Ryan C. Prager, Julia Dshemuchadse*
4:30 Paper 525e: Self-Assembly Templates for Two-Dimensional Colloidal Crystals Derived from Symmetry — ***Nathan Mahynski***, *Vincent K. Shen*
4:45 Paper 525f: Free Energy Contributions to Template-Assisted Self-Assembly of Sub-10 Nm Particles from Steered Molecular Dynamics Simulations— *Zhen Luo,* ***Shafigh Mehraeen***
5:00 Paper 525g: Parallel Bias Method for Free Energy Study of Colloidal Clusters — ***Shanghui Huang***
5:15 Paper 525h: Understanding Sequence-Dependent DNA Dynamics through Self-Associative Machine

Learning and Temperature-Jump Spectroscopy— ***Mike Jones***, *Brennan Ashwood, Andrei Tokmakoff, Andrew Ferguson*

5:30 Paper 525i: Hierarchical Self-Assembly of Thermo-Responsive Nanomaterials from Lipidated Disordered Proteins — ***Nathena Murray***, *Isabelle Tawyer, Jingjing Ji, Davoud Mozhdehi, Shikha Nangia, Md Shahadat Hossain*

5:45 Paper 525j: Exploring the Role of Lipid Tail Length on the Structure of Self-Assembled Stratum Corneum Lipids — ***Chloe Frame***, *Parashara Shamaprasad, Chris R. Iacovella, Annette Bunge, Clare McCabe*

(526) Drug Delivery for Regenerative Medicine

Wednesday, Nov 10, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 108

Michael Gower, Co-Chair
Gulden Camci-Unal, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

3:30: Break

3:48 Paper 25f: Continuous Low-Intensity Ultrasound Rescues Chondrogenesis of Mesenchymal Stromal Cells By Inhibiting NFκB Activation and Preserving Mitochondrial Potential — *Sarayu Bhogoju,* ***Anuradha Subramanian***, *Shahid Khan*

4:06 Paper 526a: Development of Phosphatidylserine Presenting Particles for Targeting Macrophages in Muscle Regeneration — ***Kidochukwu Atube***, *Christopher Isely, Candice Cheung, Michael Gower*

4:24 Paper 526b: Stimulus-Responsive Antioxidant Drug Crystals and Their Health and Ecological Implications — ***Ryan Miller***, *Byoungsoo Kim, Youngsam Kim, Chang Gyun Park, Young Jun Kim, Hyunjoon Kong*

4:42 Paper 526c: Intracellular Delivery of Antibodies for Selective Cell Signaling Interference — ***Rebecca Hershman***, *Yamin Li, Feihe Ma, Qiaobing Xu, James Van Deventer*

5:00 Paper 526e: ATRA-Loaded PLG Microparticles to Direct Macrophage Regenerative Function — ***Candice Cheung***, *Griffin Carter, Michael Gower*

5:18 Paper 526g: Leveraging Particle Size, Shape, and Deformability for Enhanced Drug Targeting in Acute and Chronic Inflammatory Diseases (Invited Speaker) — ***Lola Eniola-Adefeso***

(527) IDEAL Featured Session: A Conversation on Equity, Diversity, and Inclusion

Wednesday, Nov 10, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 203

Lucas Landherr, Chair

Sponsored by: Engineering for Inclusion

3:30: Introductory Remarks

3:35 Paper 527a: From Pledges to Practice: Turning Commitments into Action to Create More Inclusive Institutions — ***Karl Reid***

4:10: Panel Discussion: Melissa Postlewaite, DORIC; Tony Butterfield, LGBTQ+ and Allies; Karen Romero, MAC; and Caryn Heldt, WIC

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

Wednesday, Nov 10, 3:30 PM
Sheraton Back Bay, Commonwealth

Feng Jiao, Co-Chair
Hui Xu, Co-Chair
Ian McCrum, Co-Chair

Sponsored by: Electrochemical Fundamentals

3:30 Paper 528a: Studying Stability: An Investigation of Metal to Insulator Transition Induction in Strontium Iridate Perovskites for Electrochemical Water Splitting — ***Jane Edgington***, *Linsey Seitz*

3:45: Break

4:00 Paper 528c: Ionic Liquid Composite Electrocatalysts for the Oxygen Reduction Reaction in PEM Fuel Cells — ***Ramchandra Gawas***, *Maureen Tang, Joshua Snyder*

4:15 Paper 528d: Is Potential of Zero Charge a Causal Descriptor for Solvent Dynamics in the Reversible Hydrogen Electrode? — ***Luis Rebollar***, *Saad Intikhab, Suihao Zhang, Huiqiu Deng, Zhenhua Zeng, Joshua Snyder, Maureen Tang*

4:30 Paper 528e: Probing the Mechanism of Water Reduction in the Context of Thermodynamically Non-Ideal Blended Electrolytes — ***Kindle Williams***, *Aditya Limaye, Trent Weiss, Karthish Manthiram*

4:45 Paper 528f: The Role of Hydrogen Intercalation in the Kinetics of Hydrogen Evolution on WO_3 — ***Evan Miu***, *Giannis Mpourmpakis, James R. McKone*

5:00 Paper 528g: Electrocatalysis Under Cover: Enhanced Hydrogen Evolution Reaction Via Defective Graphene-Covered Pt(111) — ***Arthur J. Shih***, *Nakkiran Arulmozhi, Marc T.M. Koper*

5:15 Paper 528h: *In Situ* Identification of the Electrocatalytic Water Oxidation Behavior of a Nickel-Based Metal–Organic Framework Nanoarray — ***Fanpeng Cheng***, ***Yang Hou***

5:30: Break

5:45 Paper 528j: A Potential-Dependent Thiele Modulus to Quantify the Effectiveness of Porous Electrocatalysts — ***Charles Wan***, *Robert Darling, Yet-Ming Chiang, Fikile R. Brushett*

(529) Foundations of Systems and Process Operations

Wednesday, Nov 10, 3:30 PM
Sheraton Back Bay, Independence Ballroom West

M M Faruque Hasan, Co-Chair
Styliani Avraamidou, Co-Chair

Sponsored by: Systems and Process Operations

3:30 Paper 529a: Global Optimization of Mathematical Models with Rational Functions Using Quadratization — ***Tanuj Karia***, *Claire Adjiman, Benoit Chachuat*

3:49 Paper 529b: Hybrid Strategy for Mathematical Programming with Complementarity Constraints — ***Saif R. Kazi***, *Mandar Thombre, Lorenz Biegler*

4:08 Paper 529c: New Piecewise Relaxation with a Logarithmic Partitioning Scheme for Quadratically Constrained Problems — ***Pedro Castro***

4:27 Paper 529d: An Implementation of Locally Feasibly Projected Sequential Quadratic Programming — ***Kevin Silmore***, *James Swan*

4:46 Paper 529e: An Efficient Solution Strategy for Solving Enterprise-Wide Multi-Period Planning and Scheduling Problems: A Case Study on a Hydrogen-Based Economy — ***Cory Allen***, *Stefanos Baratsas, Rahul Kakodkar, Marcello Di Martino, Styliani Avraamidou, C. Doga Demirhan, Clara F. Heuberger, Mark Klokkenburg, Efstratios N. Pistikopoulos*

5:05 Paper 529f: Capacity Planning with Uncertain Endogenous Technology Learning — ***Tushar Rathi***, *Qi Zhang*

5:24 Paper 529g: Robust Optimization with Hybrid First-Principles Data-Driven Models — ***Chenyu Wang***, *Matthew Wilhelm, Matthew Stuber*

5:43 Paper 529h: Reactor Network Development for Multiple Rigid Polyol Productions Under Uncertainty — ***Yunhan Wen***, *Lorenz Biegler, Maria Paz Ochoa, John Weston, Nima Nikbin, Jeff Ferrio*

(530) Immunoengineering for Cancer, Vaccines, and Autoimmunity

Wednesday, Nov 10, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 109

John Blazeck, Co-Chair
Qin Qi, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

3:30 Paper 530a: Using Hyperglycosylation to Immune-Focus Toward Conserved Influenza Hemagglutinin Epitopes — ***Dana Thornlow***, *Aaron Schmidt*

3:48 Paper 530b: Developing an Enzyme to Alleviate Adenosine-Mediated Immunosuppression in Cancer — ***Maria Rain Jennings***, *John Blazeck*

4:06 Paper 530e: Combination of Toll-like-Receptor Agonists and Inhibitors for Generation of Antigen Specific Tolerance — ***Peter Deak***, *Aaron Esser-Kahn*

4:24 Paper 530f: Annexin A5-DM1 Protein Drug Conjugate Combined with Immune Stimulation and mTOR Inhibitor Treatment of Triple-Negative Breast Cancer — ***Alexis Woodward***, *Gabriela Faria, Benjamin Southard, Roger Harrison*

4:42 Paper 530g: Decoding Antigen Recognition and Signaling (Invited Speaker) — ***Michael Birnbaum***

(531) Innovations in Concept-to-Manufacturing and Distribution II

Wednesday, Nov 10, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 201

Alexander Dowling, Chair
Fani Boukouvala, Co-Chair

Sponsored by: Next-Gen Manufacturing

3:30 Paper 531a: Comprehensive Planning of Annual Delivery Program for LNG Suppliers — ***Dnyanesh Deshpande***, ***Mohd Shahrukh***, ***Rajagopalan Srinivasan***, ***Iftekhar Karimi***

3:50 Paper 531b: A New Integrated Scheduling and Optimization Framework for Holistic Refinery Supply Chain Management — ***Li Yu***, *Qiang Xu*

4:10 Paper 531c: Integrated Load Shifting and Curtailment for Demand Response of Central Chilled Water Plants — ***Gustavo Campos***, *Yu Liu, Ahmet Palazoglu, Nael El-Farra*

4:30 Paper 531d: A Web-Based Application for Chemical Production Scheduling — ***Venkatachalam Avadiappan***, *Lucas Buttazoni, Shamik Misra, Hojae Lee, Martin Yang, Christos Maravelias*

4:50 Paper 531e: Keynote Talk - Positive Power with Negative Emissions: Flexible Ngcc Enabled By Modular Direct Air Capture (DAC) — ***Matthew Realff***, *Fani Boukouvala, Christopher W. Jones, Fanhe Kong, Ryan Lively, David Thierry, Joseph K. Scott, Howard Hendrix, Katherine Dombrowski, Darshan J Sachde, Andrew Sexton*

5:25 Paper 531f: Keynote Talk - Machine Learning of Molecular and Materials Properties at the Low-Data Limit — ***Srinivas Rangarajan***, *Huijie Tian, Bowen Li*

(532) Integrated Design of Drug Substance and Drug Product Manufacture

Wednesday, Nov 10, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 101

Pablo Rolandi, Co-Chair
Shujauddin Changi, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

3:30 Paper 532b: Manufacturing and Design of a COVID-19 Vaccine Antigen for Global Access — ***Neil Dalvie***, *Sergio Rodriguez, Andrew Biedermann, Brittany Hartwell, Lisa Tostanoski, Kawaljit Kaur, Sangeeta Joshi, David Volkin, Dan Barouch, Darrell J. Irvine, J. Christopher Love*

3:54 Paper 532c: Model Assisted Development for Downstream Processing of Therapeutic Proteins — ***Igor Gonzalez***, *Angela Moser, Rushd Khalaf*

4:18 Paper 532d: Enhanced Process Characterization through Data-Rich Experimentation and Process Modeling: Generating an Intermediate Towards Islatravir — ***Brian Wyvratt***, *Cindy Hong, Jonathan McMullen, Akasha Purohit*

4:42 Paper 532e: Impurity Tracking in Integrated Pharmaceutical Batch Processes Subject to Raw

Material Variability — ***Dana Barrasso**, Sean Bermingham*
5:06 Paper 532f: Integrated Flexibility and Controllability Analysis for the Continuous Pharmaceutical Manufacturing Process — ***Wenhui Yang**, Zhihong Yuan, Bingzhen Chen*

(533) KIChE-US Chapter Open Forum (Invited Talks)

Wednesday, Nov 10, 3:30 PM
Sheraton Back Bay, Republic Ballroom A

Su Ha, Chair
Younjin Min, Chair
Tae-Sik Oh, Co-Chair
Jay Park, Co-Chair
Dongjin Seo, Co-Chair

Sponsored by: International Committee

3:30: Welcoming Remarks
3:40 Paper 533a: Surface Science - Nexus of Tribology, Glass Science, and Plant Biology — ***Seong H. Kim***
4:00 Paper 533b: High-Performance Chiral Organic Optoelectronics Using Supramolecular Chirality — ***Joon Hak Oh***
4:20 Paper 533c: Toward Single Atom Catalysis for Environmental Application— ***Jaehong Kim***
4:40 Paper 533d: Orientation of Biomaterial Based Liquid Crystal Phases and Its Application — ***Dong Ki Yoon***
5:00: KIChE US Chapter Award Ceremony
5:20 Paper 533e: Engineering Vesicles Made from Recombinant Proteins Towards Synthetic Cells — ***Yeongseon Jang***
5:40 Paper 533f: Process-Structure-Property Relationships of Stimuli-Responsive Composite Hydrogels — ***Jinhye Bae***

(534) Membrane Modeling and Simulation II

Wednesday, Nov 10, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 304

Xianghong Qian, Co-Chair
Nitish Mittal, Co-Chair

Sponsored by: Membrane-Based Separations

3:30 Paper 534a: Reconciling the Pore Flow and Solution-Diffusion Description of Swollen Membrane Transport — ***Varun Hegde**, Todd Squires, Michael F. Doherty*
3:45 Paper 534b: A Critical Comparison of Numerical Methods for Solving Coupled Multicomponent Fluxes for Complex Mixtures across Asymmetric Membranes — ***Dylan Weber**, Chau-Chyun Chen, Joseph K. Scott*
4:00 Paper 534f: Modeling of UF Performance in Pretreatment of Seawater RO Feedwater Using Neural Network with Evolutionary Algorithm and Bayesian Binary Classification — *Yang Zhou, **Yoram Cohen**, Muhammad Bilal, Han Gu, Panagiotis D. Christofides*
4:15 Paper 534g: Capturing CO_2 Via Fixed-Site-Carrier Polyvinylamine/Matrimid Facilitated Transport Membrane — ***Wrya Mohammadi Aframehr**, **Banfsheh Moki***
4:30 Paper 487g: Material Properties and Water Transport of Nanofiltration Membranes at Different pH Using Molecular Dynamics — ***Suwei Liu**, Saahir Ganti-Agrawal, Sinan Keten, Richard Lueptow*
4:45 Paper 487h: Finite-Size Effects in Molecular Dynamics Simulations of Ion Transport through Nanoporous Membranes — ***Brian Shoemaker**, Amir Haji-Akbari*

(535) Membranes for Electrochemical Conversions and Applications II

Wednesday, Nov 10, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 301

Winston Ho, Co-Chair
Peter N. Pintauro, Co-Chair

Sponsored by: Membrane-Based Separations

3:30 Paper 535a: Some Features of Ion Exchange Membranes in Complex Environments for Electrochemical Conversions — ***Thomas Zawodzinski**, Jing Peng, Kun Lou, Gabriel A. Goenaga*
4:00 Paper 535b: Molecular Engineering of Anion-Conducting Polymers for Electrochemical Energy Conversion Technologies — ***Chulsung Bae***
4:30 Paper 535c: New Membranes for Solar Fuels Systems — ***Daniel Miller**, Sarah Dischinger, Shubham Gupta, Blaine Carter*
5:00 Paper 535f: CO_2–CO Energy Conversion Cycle Enabled By a CO_2-Selective Membrane — ***Ruizhi Pang**, Yang Han, Winston Ho*

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

Wednesday, Nov 10, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 107

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

Sponsored by: Food

3:30 Paper 536a: Prebiotic Control of Microbial Communities with Human Milk Oligosaccharides — *Fatima Enam, Kelsey Dyball, **Thomas J. Mansell***
3:48 Paper 536b: Predictive Analytics for Irritable Bowel Syndrome Diagnosis and Management — *Brianna Acosta, Kiana Ramirez, **Kirti Yenkie***
4:06 Paper 536c: Identification of Unique Microbiomes Associated with Harmful Algal Blooms in Ohio River — ***Yu Zhang**, Maobing Tu*
4:24 Paper 536d: Insights into Bacterial Secondary Metabolism in Plant-Associated Ecosystems — ***Qiqi Tian**, Huimin Zhao*
4:42 Paper 536e: Biomanufacturing of Omega-3 Eicosapentaenoic Acid from Waste Cooking Oil By Metabolic Engineered Yeast *Yarrowia Lipolytica* — ***Na Liu**, Ya-Hue Soong, Andrew Olson, Dongming Xie*
5:00 Paper 489a: Creating Stable Mutants in the Plant Growth-Promoting Polyploid *Rhodopseudomonas Palustris* CGA009 — ***Cheryl Immethun**, Rajib Saha*
5:18 Paper 536g: [Invited Keynote] Towards More Accurate Models of Microbiome Metabolism: Integrating Theory and Data — ***Siu Hung Joshua Chan***

(537) Modeling, Control, and Optimization of Energy Systems II

Wednesday, Nov 10, 3:30 PM
Sheraton Back Bay, Back Bay Ballroom D

Calvin Tsay, Chair
Corey James, Co-Chair

Sponsored by: Systems and Process Control

3:30 Paper 537a: Modeling and Optimization of a Novel Solar Parabolic Trough Plant Used for Industrial Process Heat That Utilizes Flexible Heat Integration— ***Jake Immonen**, Kasra Mohammadi, Kody Powell*
3:49 Paper 537b: Moving Horizon Estimation for Heat Exchanger Processes— ***Junyao Xie**, Lu Zhang, Stevan Dubljevic*
4:08: Break
4:27 Paper 537d: Multi-Objective Economic Model Predictive Control for Heat Pump Water Heaters for Cost and Greenhouse Gas Emission Optimization — *Yue Zhang, Caton Mande, **Matthew Ellis***
4:46 Paper 537e: Simultaneous Optimization of Flow Distribution and Cleaning Schedule for Heat Exchanger Networks Subject to Maintenance Constraints— ***Parag Patil**, **Babji Srinivasan**, **Rajagopalan Srinivasan***
5:05 Paper 537f: Multi-Objective Stochastic Optimization for Hybrid Renewable Energy-Based Industrial Symbiosis Network — ***P S Pravin**, Manu Suvarna, Xiaonan Wang*
5:24 Paper 537g: Modeling Hierarchical Control Strategies, Header Balances and Tiered Pricing for Real-Time Optimization of Industrial Processes — ***Rahul Bindlish***
5:43 Paper 537h: Model Predictive Control of Integrated Energy and Chemical Manufacturing Systems — ***Davood Babaei Pourkargar***

(538) Modeling of Interfacial Systems

Wednesday, Nov 10, 3:30 PM
Sheraton Back Bay, Back Bay Ballroom A

Dmitry Kopelevich, Chair
Manuela Ayee, Co-Chair
Patricia Taboada-Serrano, Co-Chair

Sponsored by: Interfacial Phenomena

3:30 Paper 538a: Molecular Simulation of Cellulose Nanomaterials Near Montmorillonite Clays — *Andres Vodopivec, **Francisco Hung***
3:45 Paper 538c: Molecular Dynamics Study of the Biophysical Consequences of Dietary Fish Oil Incorporation into Model Membranes — ***Manuela Ayee**, Brendan Bunker, Jordan De Groot*
4:00 Paper 538d: Dynamic Molecular Switching for Environmentally Adaptive Surfaces — ***Nicholas C. Craven**, Chris R. Iacovella, G. Kane Jennings, Clare McCabe*
4:15 Paper 538e: DLVO Energy Landscape of a Janus Particle Near a Boundary — *Siddharth Rajupet, Aidin Rashidi, **Christopher Wirth***
4:30 Paper 538g: Towards a Predictive Coarse-Grained Model for Computational Design of Bioadhesives — ***Alejandro Gallegos**, Jianzhong Wu*
4:45 Paper 538h: Generalized Langmuir Isotherm Addresses Spreading Pressure Dependency of Modified Ideal Adsorbed Solution Theory — *Pradeep Vyawahare, **Usman Hamid**, Michael D. Sees, Chau-Chyun Chen*
5:00 Paper 538i: Understanding That the H-Bonding Network Controls Se Oxoanion Adsorption on Metal Oxides for Drinking Water Remediation – a Density Functional Theory Study — ***Srishti Gupta**, Anh Nguyen, Christopher L. Muhich*
5:15 Paper 538j: Experimental and CFD Modeling of Sodium Alginate Droplets Impacting Onto Immiscible Deep Liquid Surface — ***Zhizhong Ding**, Chengmin Chen, Shashank Tiwari, Krishnaswamy Nandakumar*
5:30 Paper 640a: Modeling Linear Rheology of Nanoparticle-Enhanced Viscoelastic Fracturing Fluids for Unconventional Reservoirs — ***Silabrata Pahari**, Mustafa Akbulut, Joseph Kwon*

(539) Molecular Simulations for Designing Adsorbents and Adsorption Processes I

Wednesday, Nov 10, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 305

Alexander Neimark, Chair
Daniel Siderius, Co-Chair

Sponsored by: Adsorption and Ion Exchange

3:30 Paper 539a: Molecular Simulation of Adsorption Hysteresis of n-Alkanes in Nanoporous Materials — ***Zhao Li**, Randall Snurr*
3:45 Paper 539b: Improving Computational Assessment of Water Adsorption to Enable Large-Scale Screening of Porous Materials for Water Harvesting— ***Archit Datar**, Matthew Witman, Li-Chiang Lin*
4:00 Paper 539c: Predictive Modeling of Microporous Polymeric Adsorbents of Complex Sorbates — ***Dylan Anstine**, Dai Tang, David Sholl, Coray M. Colina*
4:15 Paper 539d: Finding Selective Adsorbent Material for Selenium Oxo-Anion Removal for Water Remediation Using Ab-Initio Study with Hybrid Solvent Method. — ***Srishti Gupta**, Anh Nguyen, Christopher L. Muhich*
4:30 Paper 539f: Modeling Hydrocarbons Adsorption in Amorphous Nanoporous Carbonaceous

Materials — ***Nicholas Corrente***, *Elizabeth Hinks, Aastha Kasera, Peter Ravikovitch, Alexander Neimark*
4:45 Paper 539g: Calculation and Analysis of RAST Activity Coefficients for Ethanol/Water Adsorption in All-Silica Zeolites — ***Anne Le***, *Peng Bai*
5:00 Paper 539h: Modeling the Adsorption Behavior in Irmofs Using Monte Carlo Simulations — ***Saumil Chheda***, *Roshan Ashokbhai Patel, Laura Gagliardi, Joern Siepmann*
5:15 Paper 366b: Molecular Modeling and Adsorption Characterization of Micro-Mesoporous Kerogen Nanostructures — ***Shivam Parashar***, *Peter Ravikovitch, Alexander Neimark*

(540) New Characterization, modeling, and Processing of Nanocomposites

Wednesday, Nov 10, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 209

Mohammad Hassan, Chair
Kenan Song, Co-Chair
Luyi Sun, Co-Chair

Sponsored by: Composites

3:30 Paper 540a: Influence of Natural Gas Composition on Reserve Estimation in Carbonates: Theoretical and Experimental Investigations — *Ibnelwaleed Hussein,* ***Ibnelwaleed Hussein***, *Giuliano Carchini, Ahmed Kasha, Ahmad Sakhaee-Pour, Golibjon Berdiyorov*
3:43 Paper 540b: Generating Realistic 3D Volumes to Mimic Pore Structures in Unconventional Reservoir Rocks — ***Qiushi Sun***, *Shannon Eichmann*
3:56 Paper 540c: Efficiencies and Performance of Commercial and New Oilfield Antiscalants for Calcium Carbonate Inhibition — ***Ali Alshami***, *Trevor Taylor, Nadhem Ismail*
4:09 Paper 540d: Vertically Oriented Nanoporous Block Copolymer Membranes for Oil-Water Separation and Filtration — ***Alamgir Karim***, *Khadar Shaik, Kshitij Sharma, Maninderjeet Singh, Ali Ammar, Mohammad Hasan, Deepalekshmi Ponnamma, Samer Adham, Mariam Al-Maadeed*
4:22 Paper 540e: *Pilot-Scale Investigation of Cellulose Triacetate Hollow Fiber Forward Osmosis Membrane for Osmotic Concentration of Real Industrial Effluent* — *Rem Jalab,* ***Mustafa Nasser***, *Abdelrahman Babiker, Joel Minier-Matar, Samer Adham*
4:35 Paper 540f: Role of CO_2 Adsorption for Enhanced Gas Recovery in Carbonate Rocks: Experimental and Simulation Analysis — *Ahmed Hamza, Giuliano Carchini, Ibnelwaleed Hussein, Mohammed Al-Marri, Mohamed Mahmoud,* ***Reyad Shawabkeh***
4:48 Paper 540g: Inferring Effective Interphase Properties in Composites Reinforced with Randomly Distributed Spherical Particles — ***Joshua Arp***, *John Nicholson, Joseph Geddes, Andrew Brown, Sez Atamturktur, Christopher Kitchens*
5:01 Paper 540h: Industrial Wastewater Treatment Using Porous Nanocomposite Membranes — ***Mohammad Hassan***, *Ali El-Samak, Deepalekshmi Ponnamma, Samer Adham, Yara Hany, Mariam Al-Maadeed, Ali Ammar, Alamgir Karim*
5:14 Paper 540i: Multi-Technique Porosity and Pore Size Distribution Comparisons for Source Rocks — ***Shannon Eichmann***, *David Jacobi, Poorna Srinivasan, Kevin Kenga, Mohammed Khan, Fabian Duque, Felix Oyarzabal*
5:27 Paper 540j: Evaluating the Performance of Ni-P-ZrO_2 Nanocomposite Coatings Fabricated through Pulse Electrodeposition. — ***Abdul Shakoor***, *Mostafa Sliem, Osama Fayyaz, Khuram Shahzad*
5:40 Paper 540k: Novel Method of Fabricating Reverse Osmosis Membranes for Seawater Desalination — ***Dr. Syed Zaidi***

(541) Next-Gen Manufacturing in Pharma, Food, and Bioprocessing II

Wednesday, Nov 10, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 202

Maria Papathanasiou, Chair
Manjiri Moharir, Co-Chair

Sponsored by: Next-Gen Manufacturing

3:30 Paper 541a: Model-Based Investigation of Upstream CHO Cell Culture Process for Production of Monoclonal Antibodies with Desired N-Linked Glycosylation — ***Ou Yang***, ***Jayanth Venkatarama Reddy***, ***Katherine Raudenbush***, *Aron Gyorgypal, Shishir Chundawat, Marianthi Ierapetritou*
3:53 Paper 541b: Next-Generation Vaccines and Therapeutics: Towards Resilient Pharmaceutical Supply Chains — ***Miriam Sarkis***, *Nilay Shah, Maria Papathanasiou*
4:16 Paper 541c: Systematic Decomposition & Evaluation of a Process Design Space for Monoclonal Antibody (mAb) Manufacturing — ***Johann Kaiser***, *Maria-Ona Bertran, Janus Krarup, Manuel Pinelo, Ulrich Krühne, Deenesh K. Babi*
4:39 Paper 541d: Keynote Talk: Integrated Quality By Design in (Bio)Pharmaceutical Manufacturing — ***Richard D. Braatz***, *Moo Sun Hong, Amos E. Lu, Weike Sun*
5:14 Paper 541e: Keynote Talk: An *in silico* approach for Monoclonal Antibody (mAb) Process Research & Early Development — ***Johann Kaiser***, *Maria-Ona Bertran, Janus Krarup, Manuel Pinelo, Ulrich Krühne, Deenesh K. Babi*

(542) Particle Formation and Crystallization Processes from Liquids, Slurries, and Emulsions

Wednesday, Nov 10, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 302

Fredrik Nordstrom, Chair
Mohammad Azad, Co-Chair
Shankali U. Pradhan, Co-Chair

Sponsored by: Crystallization and Evaporation

3:30: Welcoming Remarks
3:33 Paper 542a: A Deep Learning Approach for Chord Length Distribution Modeling of Two-Dimensional Crystals — ***John Tsortos***, *Georgios Makrygiorgos, Giovanni Maria Maggioni, Ali Mesbah*
3:54 Paper 542b: Handling and Solid-State Method Development for Improved Isolation of Molecules with Complex API Structures — ***Brian Linehan***
4:15: Break
4:36 Paper 542d: Hollow Crystal Formation through a Novel Ripening Mechanism in Crystallization — ***Fredrik Nordstrom***, *Yongjian Wang, Huayu Li, Michelle Raikes, Brian Linehan, John Robson*
4:57 Paper 542e: Crystallization Engineering for the Robust Manufacturing of Islatravir Using SINTAX (shear-induced nucleation and thermal annealing crystallization) — ***Thomas Kwok***, *Eric Sirota*
5:18 Paper 542f: Evaluation of Liquid-Liquid Phase Separation and Spinodal Boundaries Using a Continuous-Flow Microfluidic Mixer — ***Paria Coliaie***, *Moussa Boukerche, Manish Kelkar, Marianne Langston, Chengxiang Liu, Neda Nazemifard, Daniel Patience, Dimitri Skliar, Nandkishor K. Nere, Meenesh Singh*
5:39 Paper 542g: Molecular Simulations Reveal Underlying Mechanism of Cooling and Antisolvent Crystallization to Predict the Polymorphism and Growth of Organic Crystals — ***Anish Dighe***, *Prem Kumar Reddy Podupu, Paria Coliaie, Meenesh Singh*

(543) Plenary Session: Computational Molecular Science and Engineering Forum (Invited only)

Wednesday, Nov 10, 3:30 PM
Marriott Copley Place, Salon J/K

Sapna Sarupria, Chair
Jim Pfaendtner, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

3:30 Paper 543a: Synergistic Integration of Coarse-Grained Models, PRISM Theory, and Molecular Simulations for Design and Characterization of Macromolecular Materials — ***Arthi Jayaraman***
4:10 Paper 543b: Computational Exploration of High-Chi Block Oligomers— ***Joern Siepmann***
4:30 Paper 543c: Molecular and Data-Centric Modeling of Nanoparticle Interactions with Biological Interfaces — ***Reid Van Lehn***
5:10 Paper 543d: Mechanisms of Ion Transport in Polymeric Ionic Liquids— ***Venkat Ganesan***
5:30 Paper 543e: Elucidating Chemical Evolution in Shocked Materials— ***Rebecca Lindsey***

(544) Process Design in Energy and Sustainability

Wednesday, Nov 10, 3:30 PM
Sheraton Back Bay, Back Bay Ballroom C

Apoorva Sampat, Co-Chair
Kirti Yenkie, Co-Chair
Matthew Stuber, Co-Chair

Sponsored by: Systems and Process Design

3:30 Paper 544a: Optimization Framework for the Electroreduction of CO_2 into Chemicals — ***Ana Somoza Tornos***, *Omar J. Guerra, Wilson A. Smith, Bri-Mathias Hodge*
3:51 Paper 544b: Material Property Targets for Emerging Adsorptive Water Treatment and Resource Recovery Systems — ***Elvis Eugene***, *William Phillip, Alexander Dowling*
4:12 Paper 544c: Integrated Waste-to-Energy and Energy Management Platform: A Demonstration in an Eco-Industrial Park — ***Lanyu Li***, *Laura Ong, Mei Qi Lim, Markus Kraft, Xiaonan Wang*
4:33 Paper 544d: Design and Integration of Thermal Energy Storage Systems for Power Plants — ***Mengdi Li***, *Akhilesh Gandhi, Manali S. Zantye, M M Faruque Hasan*
4:54 Paper 544e: A Multiscale Electro-Chemical Model for Simulating Dendrite Formation in Lithium-Ion Batteries — ***Hyeonggeon Lee***, *Niranjan Sitapure, Maria Stefany Angarita-Gomez, Perla B. Balbuena, Sungwon Hwang, Joseph Kwon*
5:15 Paper 544f: Computationally Efficient Distillation Energy Targeting Model for Superstructure-Based Process Synthesis — ***Joonjae Ryu***, *Christos Maravelias*
5:36 Paper 544g: Dynamic Simulation of an Ammonia Synthesis Plant Fed By Stranded Natural Gas in Aspen Hysys — ***Laron Burrows***, *George Bollas*

(545) Process Intensification and Modular Manufacturing: Modular/Advanced Manufacturing

Wednesday, Nov 10, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 208

Paul Yelvington, Chair
Fereshteh Farzad, Co-Chair

Sponsored by: Process Intensification & Modular Chemical Processing

3:30 Paper 545a: Development and Commissioning of a Modular and Integrated Apparatus for the Quasi-Continuous Production of Crystalline Particles — ***Timo Dobler***, *Marco Gleiss, Hermann Nirschl*
3:50 Paper 545b: Scalable Modular Manufacturing of Crystals with Improved Uniformity — ***Mo Jiang***
4:10 Paper 545c: Self-Heat Recuperative Heat Circulation System By Using Heat Pump Module — ***Atsushi Tsutsumi***
4:30 Paper 545d: Localized Heating of Microreactors for Alkane Dehydrogenation — ***Abhinav Malhotra***, *Weiqi Chen, Weiqing Zheng, Pedro Plaza-Gonzalez, Jose M. Catala-Civera, Dionisios Vlachos*

(546) Proteins in Biomedical and Biomaterials Engineering

Wednesday, Nov 10, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 110

John Blazeck, Chair
Jason Boock, Co-Chair

Sponsored by: Bioengineering

3:30 Paper 546a: Protein-Engineered Block Copolymers for Water-Responsive Actuation — ***Jacob Kronenberg***, *Yeojin Jung, Jason Chen, Xi Chen, Raymond S. Tu, Jin Kim Montclare*
3:48 Paper 546b: Enabling Directed Evolution in Materials Development: High-Throughput Screening of Streptavidin-Binding Proteins in Self-Assembled Solid Films — ***Melody Morris***, *Carolyn E. Mills, Justin M. Paloni, Eric A. Miller, Hadley D. Sikes, Bradley Olsen*
4:06 Paper 546c: Mechanically Dynamic Silk Protein-Based Hydrogels for Studying Fibrosis — ***Thomas Falcucci***, *Onur Hasturk, Jaewon Choi, Jugal Kishore Sahoo, Andy T. Lee, Clark T. Hung, David L. Kaplan*
4:24 Paper 546d: Preservation of Protein Stability and Activity By Confinement in Michael-Type Addition Polyethylene Glycol Hydrogels — ***Zahra Ghassemi***, *Sam Ruesing, Silviya Petrova Zustiak, Jennie Leach*
4:42 Paper 546e: Downregulation of the T7 Promoter in *E. coli* for Enhanced Production of Small Recombinant Spidroins — ***Alexander Connor***, *R. Helen Zha, Mattheos Koffas*
5:00 Paper 546f: A Novel Mechanism for Gluten Transport across the Cell Membrane: Implications for Celiac Disease, — ***Elise Loppinet***, *Chaitan Khosla*, Ruize Zhuang*
5:18 Paper 546g: Basic Principles of Tissue Transformation Technologies for Organ-Scale Molecular Imaging and Phenotyping (Invited Talk) — ***Kwanghun Chung***

(547) Stories from Biotech Start-ups-Invited

Wednesday, Nov 10, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 303

Pratik Umesh Joshi, Chair
Ranil Wickramasinghe, Co-Chair

Sponsored by: Bio Separations

3:30 Paper 547a: Industrializing Exosomes: Turning Research Breakthroughs into Clinical Candidates — ***Aaron Noyes***
4:00 Paper 547b: Sunflower Therapeutics: Starting a Public Benefit Corporation in Biotech — ***Laura Crowell***
4:30 Paper 547d: Translating Biotechnologies from the Lab to Start-up's – Three Companies, Three Paths — ***John Love***
5:00: Panel Discussion

(548) Systems Biology in Human Health and Disease

Wednesday, Nov 10, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 111

Kevin Metcalf, Chair
Shelby Mills, Co-Chair

Sponsored by: Bioengineering

3:30 Paper 548a: Characterizing Microbial Taxa and Metabolic Pathways Trends Following Microbiota Transfer Therapy in Children with Autism Spectrum Disorder and Gastrointestinal Symptoms — ***Fatir Qureshi***, *Rosa Krajmalnik-Brown, Khemlal Nirmalkar, James B. Adams, Dae-Wook Kang, Juergen Hahn*
3:48 Paper 548b: Cross-Tissue Drug Signature Predictions for Drug Repurposing — ***Panagiotis Chrysinas***, *Rudiyanto Gunawan*
4:06 Paper 548c: Single-Cell Transcriptomic Analysis of Retinal Neurons in Nine Species Facilitates Comparison of Cell Type Diversity across Evolution— ***Joshua Hahn***, *Zaid Ahmad, Shawn Koong, Karthik Shekhar, Joshua Sanes, Yi-Rong Peng, Aboozar Monavarfeshani*
4:24 Paper 548d: Elucidating Neuron-Glia Interactions in a Whole-Hemisphere Brain Slice Model of Neonatal Hypoxia Ischemia — ***Jeremy Filteau***, *Elizabeth Nance*
4:42 Paper 548e: A Transient Metabolic State in Melanoma Persister Cells Mediated By Chemotherapeutic Treatments — ***Prashant Karki***, *Vahideh Angardi, Juan Mier, Mehmet Orman*
5:00 Paper 548f: An Immunoinhibitory Glycocalyx Signature Associates with Breast Cancer Aggression — ***Kevin Metcalf***, *Mary-Kate Hayward, Eric Berens, Valerie Weaver*
5:18 Paper 548g: Engineering Cell Fate Via Cellular Reprogramming — ***Kate Galloway***

(549) Teaching Data Science to Students and Teachers III

Monday, Nov 15, 8:00 AM
Virtual, Bridging the Skills Gap in Chemical Engineering (T4)

Martha Grover, Chair
Phillip Westmoreland, Co-Chair

Sponsored by: Bridging the Skills Gap in Chemical Engineering

8:00 Paper 549a: Data Dexterity at Rensselaer — ***Juergen Hahn***, *Xun Wang, Uwe Kruger*
8:20 Paper 549b: Integrating Data Science to Chemical Engineering Curriculum Using Matlab — ***Aycan Hacioglu***, *Samvith Rao*
8:40 Paper 549c: Linking Measurements and Statistical Methodology through the Characterization of Polymeric Materials: Hierarchical Analysis of Gel Permeation Chromatography Data — ***Alison Scott***, *Nicholas Filipovic, Alexander Penlidis*
9:00 Paper 549d: Interactive Modules for Teaching Hands-on Data Science in Engineering — *Kerul Suthar, Thomas MItchell, Anna Hartwig, Jin Wang,* ***Q. Peter He***
9:20 Paper 549e: Learning Coarse-Scale ODEs/PDEs from Microscopic Data: What and How Can We Learn It from Data? — ***Seungjoon Lee***, *Georgios Psarellis, Ioannis G. Kevrekidis*
9:40 Paper 549f: From Molecular- to Plant-Scale Computational-Engineering Design: Applied Training Spanning Scales — ***Niall English***
10:00 Paper 506a: Open Source Data Science Education Materials for Chemical Engineers — ***David Beck***, *Stephanie Valleau, Caitlyn Wolf, Chad D. Curtis, Jim Pfaendtner*

(550) T&EP Graduate Student Award Session

Wednesday, Nov 10, 3:30 PM
Sheraton Back Bay, Back Bay Ballroom B

Andrej Lenert, Chair
Abhinav Malhotra, Co-Chair

Sponsored by: Transport and Energy Processes

3:30 Paper 550a: Chemical Looping Ammonia Synthesis By Activating Dinitrogen : Nitridation of Manganese — ***Wrya Mohammadi Aframehr***, *Peter Pfromm*
3:51 Paper 550b: Non-Solvent Induced Phase Separation for Designer Porous Carbon Electrodes — ***Charles Wan***, *Rémy Jacquemond, Antoni Forner-Cuenca, Yet-Ming Chiang, Fikile R. Brushett*
4:12 Paper 550c: The Role of Water in Vapor-Fed Proton-Exchange-Membrane Electrolysis — ***Julie Fornaciari***, *Samay Garg, Nemanja Danilovic, Alexis Bell, Adam Weber*
4:33 Paper 550d: A Theoretical Study on the Solvation of Lithium Ion with Asymmetric Anions for the Development of Concentrated Electrolytes for Li-Ion Batteries — ***Drace Penley***, *Stephen Vicchio, Rachel Getman, Burcu Gurkan*
4:54 Paper 550e: Organic Solvent Membrane Filtration: Rational Design of Bottlebrush Membranes — ***Pranav Ramesh***, *Mirco Sorci, Dinesh Behera, Bratin Sengupta, Surya Padinjarekutt, Miao Yu, James (Chip) Kilduff, Georges Belfort*
5:15 Paper 550f: Cell-Free Production of Isobutanol: A Completely Immobilized System — ***Matthew Wong***, *Sarah Morais, Mirco Sorci, Christopher Gasparis, Edward Bayer, Georges Belfort, Mattheos Koffas*
5:36 Paper 550g: Understanding V^{2+}/V^{3+} Reaction on Metal Electrocatalysts for Vanadium Redox Flow Batteries — ***Harsh Agarwal***, *Jacob Florian, Bryan Goldsmith, Nirala Singh*

(551) Thermophysical Properties and Phase Behavior

Wednesday, Nov 10, 3:30 PM
Marriott Copley Place, Salon C/D

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

Sponsored by: Thermodynamics and Transport Properties

3:30 Paper 551a: Area 1a Plenary: Towards the Elucidation of the Mechanism of Synthesis of Zeolites — ***Valeria Molinero***
4:10 Paper 551b: Properties and Phase Behavior of Supercooled Water from First Principles — ***Thomas Gartner III***, *Pablo M. Piaggi, Roberto Car, Athanassios Panagiotopoulos, Pablo Debenedetti*
4:25 Paper 551f: Cholesteric Blue Phase Liquid Crystal Core-Shells — ***Sepideh Norouzi***, *Jose A. Martinez-Gonzalez, Juan J. DePablo, Monirosadat Sadati*
4:40 Paper 551g: Saturation Point Calculations in Reactive Systems Based on the RAND Method — ***Fernando Medeiros***, *Erling H. Stenby, Wei Yan*
4:55 Paper 551h: A New Approach to Predicting Saturated Liquid Viscosity from MD Simulations for Transferability and Accuracy — ***Daniel Carlson***, *Thomas Knotts IV*

(553) Transitioning from Graduate School to Your Future (Panel Discussion)

Wednesday, Nov 10, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 312

Shelby Mills, Co-Chair
Victoria Muir, Co-Chair

Sponsored by: Young Professionals Committee (YPC)

(554) Turbulent, Reactive Flows and Flow Characterization

Wednesday, Nov 10, 3:30 PM
Sheraton Back Bay, Constitution A

Joseph Samaniuk, Chair
Suraj Deshpande, Co-Chair

Sponsored by: Fluid Mechanics

3:30 Paper 554a: Kinetics of Polyethyleneoxide U309 Degradation during Turbulent Drag Reduction in a Hydrodynamically Smooth 4.58 Mm ID x 180 L/D Pipe — ***Preetinder Virk***
3:47 Paper 554b: Modeling Chaotic Spatiotemporal Dynamics with a Minimal Representation Using Neural ODEs — ***Alec Linot***, *Michael Graham*
4:04 Paper 554c: Linear Versus Branched: Flow of a Wormlike Micellar Fluid Past a Falling Sphere — *Shijian Wu,* ***Hadi Mohammadigoushki***
4:21 Paper 554d: Turbulence and Interpenetrating Continua — ***Charles Petty***, *Andre Benard*
4:38 Paper 554e: Reverse Transition Routes from Inertial to Elasticity-Dominated Turbulence in Viscoelastic Taylor-Couette Flow — *Jiaxing Song, Nansheng Liu,* ***Bamin Khomami***
4:55: Break
5:12: Break
5:29 Paper 554h: Three-Phase Air-Liquid-Liquid Gravity Driven Flow from Storage Tank — ***Ranjana Rathaur***
5:46 Paper 554i: Fluorescent Particle Streak Velocimetry Applied to Fast-Flowing Suspensions — ***Han Lin***, *Brendan Blackwell, Michelle Driscoll, Jeffrey Richards*

(556) William R. Schowalter Lecture

Wednesday, Nov 10, 6:15 PM
John B. Hynes Veterans Memorial Convention Center, Ballroom B

Pablo Debenedetti, Chair

Sponsored by: Awards Committee

6:15 Paper 556a: Particle Suspensions in Elastic Fluids: From Synovial Fluid Therapy to a "Swimming Rheometer" — ***Eric S.G. Shaqfeh***, *Anika Jain, Anni Zhang, Jeremy Binagia, Laurel Kroo, Manu Prakash*

(557) Advanced Electrochemical Energy Storage Technologies II

Thursday, Nov 11, 8:00 AM
Sheraton Back Bay, Back Bay Ballroom B

Gang Wu, Chair
Ling Fei, Co-Chair

Sponsored by: Transport and Energy Processes

8:00 Paper 557a: Solid State Battery Based on PEO/PVDF-HFP Solid Polymer Electrolyte — ***Han Yu***, *Xinhua Liang*
8:25 Paper 557b: Ion Transport and Ion-Correlation in Non-Aqueous Lithium-Ion Polyelectrolyte Solutions — ***Helen Bergstrom***, *Kara Fong, Bryan McCloskey*
8:50 Paper 557d: Studying the Mechanism of the High Voltage Ce^{3+}/Ce^{4+}Redox Couple through Kinetic Measurements and Spectroscopy — ***Cailin Buchanan***, *Dylan Herrera, Bryan Goldsmith, Nirala Singh*

(558) Advances in nonlinear and surrogate optimization

Thursday, Nov 11, 8:00 AM
Sheraton Back Bay, Independence Ballroom West

Andrew Allman, Co-Chair
Yankai Cao, Co-Chair

Sponsored by: Systems and Process Operations

8:00 Paper 558a: A Novel Constrained Bayesian Optimization Method for Computationally Expensive Grey-Box Models with Composite Objective and Constraint Functions — *Congwen Lu,* ***Joel Paulson***
8:19 Paper 558b: A Unifying Abstraction for Infinite-Dimensional Optimization— ***Joshua Pulsipher***, *Weiqi Zhang, Victor M. Zavala*
8:38 Paper 558c: Exponential Decay of Sensitivity in Graph-Structured Nonlinear Programs — *Sungho Shin, Mihai Anitescu,* ***Victor M. Zavala***
8:57 Paper 558d: Learning the Structure of Optimization Problems through Stochastic Blockmodeling — ***Ilias Mitrai***, *Prodromos Daoutidis*
9:16 Paper 558e: A New Reinforcement Learning Based Bayesian Optimization Method for a Sequential Decision Making in an Unknown Environment — ***Mujin Cheon***, *Ha-Eun Byun, Jay H. Lee*
9:35 Paper 558f: A Nested Schur Decomposition Approach for Multiperiod Optimization of Chemical Process — *Noriyuki Yoshio,* ***Lorenz Biegler***
9:54 Paper 558g: Model-and-Search: A Derivative-Free Local Optimization Algorithm — ***Kaiwen Ma***, *Luis Miguel Rios, Nikolaos Sahinidis*
10:13 Paper 558h: Safe Real-Time Optimization Using Multi-Fidelity Gaussian Processes — ***Panagiotis Petsagkourakis***, *Benoit Chachuat, Antonio del Rio Chanona*

(559) Antifouling Membranes for Water Purification

Thursday, Nov 11, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 304

Steven Weinman, Co-Chair
Siamak Nejati, Co-Chair

Sponsored by: Membrane-Based Separations

8:00 Paper 559a: Flux and Antifouling Performance of Bioinspired Liquid-Infused Membranes — ***Rushabh Shah***, *Aydin Cihanoğlu, Justin Hardcastle, Caitlin Howell, Jessica Schiffman*
8:15 Paper 559b: Optimizing Ultrafiltration Membranes Surface Energy to Mitigate Fouling By Polysiloxane Grafting — ***Thien Tran***, *Xiaoyi Chen, Sarthak Doshi, Christopher M. Stafford, Haiqing Lin*
8:30 Paper 559c: Fouling of Microfiltration Membranes By Bidisperse Particle Solutions — ***Haichao Wu***, *Daniel K. Schwartz*
8:45 Paper 559g: Improvement of Oil/Water Emulsion Separation Efficiency Using Modified α-Alumina Membranes with Ludox Colloidal Silica Nanoparticles— *Anirban Ghosh,* ***Diako Mahmodi***, *Michael Miranda, Clint Aichele, Seokjhin Kim*
9:00 Paper 408b: Customized thin film composite membranes using additive manufacturing — ***Xin Qian***, *Tulasi Ravindran, Maqsud R. Chowdhury, Samuel Lounder, Asye Asatekin, Rhea Verbeke, Ivo F. J. Vankelecom, Jeffrey McCutcheon*

(560) Applied Math for Energy and Environmental Applications

Thursday, Nov 11, 8:00 AM
Sheraton Back Bay, Back Bay Ballroom D

Fernando V. Lima, Chair
Apoorva Sampat, Co-Chair

Sponsored by: Applied Mathematics and Numerical Analysis

8:00 Paper 560a: A Bayesian Method for Finding the Tolerances Around a Bi-Objective Pareto Front: Application to Electrochemical Carbon Capture Solution Chemistries — ***Jonathan Boualavong***, *Christopher Gorski*
8:19: Break
8:38 Paper 560c: Development of Computationally Efficient Dynamic Model to Estimate Consequence of Rare Events — ***Pallavi Kumari***, *Bhavana Bhadriraju, Qingsheng Wang, Joseph Kwon*
8:57 Paper 560e: What Matters and What Does Not Matter: Parametrizing Common and Sensor-Specific Information across Multiple Sensors in Chemically Reacting Systems — ***David Sroczynski***, *Felix Dietrich, Ronen Talmon, Ioannis G. Kevrekidis*
9:16 Paper 560f: Recent Advances in Kipet — ***Kevin McBride***, *Lorenz Biegler, Salvador Garcia-Munoz*
9:35 Paper 560g: A Nonsmooth Approach to Multicomponent Mass and Water Integration — ***Caroline Nielsen***, *Paul I. Barton*
9:54 Paper 560h: From Elementary Steps of Multistep Catalytic Polymer Upcycling Mechanisms to Derived Population Balance Models — ***Ziqiu Chen***, *Baron Peters, Damien Guironnet*

(561) Biological Conversions and Processes for Renewable Feedstocks

Thursday, Nov 11, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 312

Shishir Chundawat, Chair
Rebecca Ong, Co-Chair
Hasan Atiyeh, Co-Chair

Sponsored by: Sustainable Biorefineries

8:00 Paper 561a: Effects of Microporous Structure on Transient Diffusion and Adsorption of Hydrolytic Enzymes into Biomass — ***Saketh Merugu***
3:30 Paper 162f: Characterization of Cellulose Biopolymer Synthesizing Enzymes Reconstituted *in Vitro* — ***Dharanidaran Jayachandran***, *Shishir Chundawat*
8:30 Paper 561c: Lignin Valorization By Integrating Chemical Depolymerization and Microbial Funneling: New Strategies to Produce 2-Pyrone-4,6-Dicarboxylic Acid — ***Canan Sener***, *Miguel Perez, German Umana, Shamik Misra, Christos Maravelias, Steven D. Karlen, Timothy J. Donohue, Daniel R. Noguera, John Ralph*
8:45 Paper 561d: Understanding the Impact of High Solids Loadings on Deconstruction of Celf Pretreated Poplar By *C. Thermocellum* consolidated Bioprocessing (CBP) — ***Priyanka Singh***, *Evert K. Holwerda, Maria Pena, Yining Zeng, Yunqiao Pu, Christian Alcaraz, Yannick J. Bomble, Lee R. Lynd, Charles M. Cai, Charles E. Wyman*
9:00 Paper 561e: Comparison of Five Acetogens for Production of C_2 – C_6Alcohols and Acids from CO_2— *Rahul Thunuguntla,* ***Hasan Atiyeh***, *Raymond L. Huhnke, Ralph S. Tanner*
9:15 Paper 561f: System-Level Analysis of Isobutanol Production in Lignocellulosic Biorefineries — ***Arthur Eduardo Pastore De Lima***, *Brandon Paul, Christos Maravelias*

(562) Biomaterials: Graduate Student Award Session

Thursday, Nov 11, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 103

Mark Tibbitt, Chair
Rong Tong, Co-Chair
Nisarg Shah, Co-Chair
Xiaoping Bao, Co-Chair

Sponsored by: Biomaterials

8:00 Paper 562a: Graduate Student Award Session: Polymer Nanoparticle Hydrogels for Improved Cell Transplantation — ***Abigail Grosskopf***, *Gillie A. Roth, Joseph Mann, Emily Gale, Hector Lopez Hernandez, Santiago Correa, Eric A. Appel*
8:18 Paper 562b: Graduate Student Award Session: Cysteine-Conjugated Thermoresponsive Hydrogels As Mucoadhesive Intestinal Scaffolds — ***Ninad Kanetkar***, *Adam Ekenseair*
8:36 Paper 562c: Graduate Student Award Session: The Combined Influence of Viscoelastic and Adhesive Cues on Fibroblast Spreading and Focal Adhesion Organization — ***Erica Hui***, *Leandro Moretti, Thomas Barker, Steven Caliari*
8:54 Paper 562d: Graduate Student Award Session: Effects of Nanoscale Magnetite on Human Forebrain-like Tissue Development in Stem Cell-Derived Cortical Spheroids — *Elizabeth Henderson, Sonia Kiran,* ***Thien Hua***, *Zahraa Khamis, Yan Li, Qing-Xiang Amy Sang*
9:12 Paper 562e: Graduate Student Award Session: Engineering a Biocompatible Chitosan Hydrogel with Self-Healing, Adhesive and Inherent Antibacterial Properties — ***Celine Garcia***, *Rebecca Gabrilska, Kendra Rumbaugh, Wei Li*
9:30 Paper 562f: Graduate Student Award Session: Osmotic-Capillary Principles for Microfluidic Pumping and Fluid Management for Sweat Sensing Devices — ***Tamoghna Saha***, *Jennifer Fang, Sneha Mukherjee, Michael D. Dickey, Orlin D. Velev*
9:48 Paper 562g: Award Session: Impact of Collagen-like-Peptide (CLP) Triple Helix Design on CLP Melting Transition and Assembly: A Coarse-Grained Molecular Dynamics Simulation Study — ***Phillip Taylor***, *April Kloxin, Arthi Jayaraman*
10:06 Paper 562h: Graduate Student Award Session: Enhanced Granular Hydrogel Properties through Dynamic Covalent Interparticle Crosslinking— ***Victoria Muir***, *Jason A. Burdick*

(563) Biopolymers

Thursday, Nov 11, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 104

Danielle Mai, Chair
Yeongseon Jang, Co-Chair

Sponsored by: Polymers

8:00 Paper 563b: Sequence Modulates Polypeptoid Hydration Water Structure and Dynamics — ***Sally Jiao***, *Audra DeStefano, Daniela Rivera-Mirabal, Rachel Segalman, Songi Han, M. Scott Shell*
8:15 Paper 563c: Role of Charge Patterning and Hydrophobicity in Peptide-Based Complex Coacervates — ***Arvind Sathyavageeswaran***, *Jason Madinya, Charles Sing, Sarah L. Perry*

8:30 Paper 563d: Impact of Collagen-like-Peptide (CLP) Triple Helix Design on CLP Melting Transition and Assembly: A Coarse-Grained Molecular Dynamics Simulation Study — ***Phillip Taylor***, *April Kloxin, Arthi Jayaraman*
8:45 Paper 563e: Controlled Alignment of Collagen and its Influence on the Proliferation of Human Schwann Cells — ***Homa Ghaiedi***, *Luis Carlos Pinzon-Herrera, Jorge Almodovar, Karthik Nayani*
9:00 Paper 563f: Opto-Chemical Characterization and Determination of Nanostructural Organization in Complex Leafhopper Brochosome Protein Assemblies — ***Gabriel Burks***, *Progna Banerjee, Marianne Alleyne, Mostafa Nassr, Sarah Bialik, Elizabeth Bello, Benny D. Freeman, Jeffrey E. Barrick, Delia Milliron, Charles M. Schroeder*
9:15 Paper 563h: Mucus: Cactus-like Conformations of Associative Polymers— ***Scott Danielsen, PhD***, *Michael Rubinstein*
9:30 Paper 563g: Barrier Coatings Derived from Cellulose and Chitin — ***J Carson Meredith***, *Meisha L. Shofner, Yue Ji, Zeyang Yu*
10:00 Paper 563a: Engineering Electrostatic Interactions between Proteins and Biopolymers for Intracellular Phase Separation — *Vivian Yeong, Jou-wen Wang, Justin Horn,* ***Allie Obermeyer***
10:15 Paper 563i: Kinetics of Soy Protein Adsorption at the Fluid Interface: Interfacial Rheology — ***Farshad Nazari***, *Mohammad Reza Rahimpour*

(564) Catalyst Design, Synthesis, and Characterization III - Structure/Activity relationships studies

Thursday, Nov 11, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 205

George Tsilomelekis, Chair
Konstantinos Alexopoulos, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

8:00 Paper 564b: Nanoparticle Size Effects on Phase Stability for Molybdenum and Tungsten Carbides — ***Anukriti Shrestha***, *Xutao Gao, Jason Hicks, Christopher Paolucci*
8:20 Paper 564c: Molten Salt Synthesis of NiO, MgO, and Their Mixed Oxides: Designing New Methods to Control Crystal Morphology — ***Mariano D. Susman***, *Hien N. Pham, Xiaohui Zhao, Raffaele Cheula, David West, Sivadinarayana Chinta, Matteo Maestri, Praveen Bollini, Abhaya K. Datye, Jeffrey Rimer*
8:40 Paper 564e: Enhancing Hydrophobicity and Catalytic Activity of Nano-Sn-Beta for Alcohol Ring Opening of Epoxides through Post-Synthetic Treatment with Fluoride — ***Alexander Spanos***, *Aamena Parulkar, Nicholas Brunelli*
9:00 Paper 564f: Steering CO_2 Hydrogenation Towards C-C Coupling to Hydrocarbons Using Porous Organic Polymer/Metal Interface — ***Chengshuang Zhou***, *Arun Asundi, Emmett Goodman, Jiyun Hong, Baraa Werghi, Adam Hoffman, Stacey F. Bent, Simon Bare, Matteo Cargnello*
9:20 Paper 509e: Rational Bimetallic Catalyst Synthesis By Electroless Deposition Method and Application for Renewable Chemical Production— ***Weijian Diao***
9:40 Paper 509bv: A General Nanocasting Encapsulation Strategy Promotes High-Temperature Stability of Metal Catalysts. — ***Aisulu Aitbekova***, *Chengshuang Zhou, Adam Hoffman, Simon Bare, Philipp Plessow, Matteo Cargnello*

(565) Charged and Ion-Containing Polymers 2

Thursday, Nov 11, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 105

Whitney Loo, Chair
Hee Jeung Oh, Co-Chair
Samanvaya Srivastava, Co-Chair
Xiaoxue Wang, Co-Chair

Sponsored by: Polymers

8:00 Paper 565a: New Insights into the Mechanism of Action of Cationic π-Conjugated Polyelectrolytes Against Bacteria — ***Ehsan Zamani***, *Shyambo Chatterjee, Shudipto K. Dishari*
8:15 Paper 565b: Molecular Conformation for Conjugated Polymers in Solution— ***Xiaodan Gu***, *Zhiqiang Cao*
8:45 Paper 565c: Influence of Small Ions on Composition and Viscoelasticity of Polyelectrolyte Complexes — *Divya Iyer, Vaqar M. S. Syed,* ***Samanvaya Srivastava***
9:00 Paper 565d: Materials Processing Using Complex Coacervates — ***Isaac Ramirez Marrero***, *Luke Boudreau, Bernhard von Vacano, Rupert Konradi, Rainer Gutzler, Sarah L. Perry*
9:15 Paper 565f: Obtaining Specific Ion Binding Free Energies on Polyelectrolytes Using Atomistic Molecular Dynamics Experiments — *Wen-de Tian,* ***Mohsen Ghasemi***, *Ronald Larson*
9:30 Paper 565g: Polyelectrolytes Dynamics and Rheology, in a Pinch — *Leidy N. Jimenez, Chenxian Xu, Jelena Dinic,* ***Vivek Sharma***
9:45 Paper 565h: Charge Regulation of Weak Polyelectrolytes in Inhomogeneous Solutions — ***Alejandro Gallegos***, *Gary Min Chiang Ong, Jianzhong Wu*
10:00 Paper 565i: Solventless Synthesis of pH-Responsive Polymer Sponge Coatings — ***Stacey Bacheller***, *Malancha Gupta*
10:15 Paper 565e: Physical Property Scaling Relationships for Polyelectrolyte Complex Micelles — ***Alexander Marras***, *Jeffrey R. Vieregg, Matthew V. Tirrell*

(566) Climate Change and Engineering Sustainability

Friday, Nov 19, 8:00 AM
Virtual, Sustainable Engineering Forum (23)

Simona Liguori, Chair
Raymond Smith, Co-Chair

Sponsored by: Sustainability Science and Engineering

8:00: Break
8:25 Paper 566b: Seawater-Air-Sunlight Based Industrial Clusters for Carbon Dioxide Utilization — *Elizabeth Abraham,* ***Farah Ramadan***, *Dhabia Al-Mohannadi*
8:50 Paper 566c: The Effect of Cultivation History on the Growth Phenotype of a Type I Methanotroph — *Kiumars Badr, Matthew Hilliard,* ***Alisabeth Bradford***, *Q. Peter He, Jin Wang*
9:15 Paper 566d: Improving Global Nitrogen Cycle Management Via Mechanochemical High Efficiency Urea Cocrystal Fertilizer Material Synthesis and Utilization — ***Manoj Silva***, *Jonas Baltrusaitis*
9:40: Break
10:05 Paper 566f: European Path Towards Carbon Neutrality By 2050— ***Roghayeh Dejan***, *Caroline Ganzer, Niall Mac Dowell*

(567) CO_2 Capture By Adsorption I

Wednesday, Nov 10, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 305

F Handan Tezel, Chair
Masoud Jahandar Lashaki, Co-Chair

Sponsored by: Adsorption and Ion Exchange

8:00 Paper 567c: Design of Metal Organic Frameworks (MOFs) with Enhanced CO_2 Adsorption Using Machine Learning — ***Abhishek Sose***, *Samrendra Singh, Karteek K. Bejagam, Sanket Deshmukh*
8:25 Paper 567e: Impact of Controlled Morphology and Defect Density on Gas Sorption in a MOF for Direct Air Capture of Carbon Dioxide — *Xakin Ramirez Isunza, Connor Farrell, Brittany Bonnett, Amanda J. Morris,* ***Stephen Martin***
8:50 Paper 567g: Tuning CO_2 Binding in Metal-Organic Framework Materials through Control over Metal Identity and Oxidation State — ***Mengying Li***, *Jacklyn Hall, Kevin Fleming, Hakan Demir, Lars Grabow, Praveen Bollini*
9:15 Paper 567f: Evaluating Degradation of CO_2 Adsorbents in BECCS Processes — ***Hannah Holmes***, *Robert D. Schreck V, Wenting Sun, Matthew Realff, Ryan Lively*
9:40 Paper 567a: Development of Large Scale PSA Processes for CO_2 Capture with O_2 Removal Capability — ***Huan Jiang***, *Armin Ebner, James A. Ritter*

(568) Crystallization Process Development

Thursday, Nov 11, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 302

Daniel Green, Chair

Sponsored by: Crystallization and Evaporation

8:00: Welcoming Remarks
8:03 Paper 568a: Cephalexin and Amoxicillin Crystal Shape Modification By Manipulating the Supersaturation and Wet Milling — ***Hossein Salami***, *Patrick Harris, Andreas Bommarius, Martha Grover, Ronald Rousseau*
8:24 Paper 568b: Accelerated Early-Stage Enabling API Crystallization Process Development and Scale-up — ***Ryan Ellis***, *Moussa Boukerche, Collin Morris, Michael Lesslie, Jie Chen, James Stambuli, Nandkishor K. Nere*
8:45 Paper 568c: Development and Scale-up of a Crystallization Process for a Kinetically-Unfavorable Polymorph — ***Paul Larsen***, *Navraj Hanspal, Nicole Hough, Christian Lowe, Yamini Krishnan, Patrick McGough, Abraham Schuitman, Joseph Wei*
9:06: Break
9:27 Paper 568e: Acid-Catalyzed Esterification Governs the Chain Elongation and the Oriented Attachment in Cof-5 Synthesis — ***Rajan Bhawnani***, *Anish Dighe, Santanu Chaudhuri, Meenesh Singh*
9:48 Paper 568f: Enabling a Selective Dissolution Scheme for the Removal of Fines in Crystallization with a Hydrocyclone: Modeling and Experimental Validation — ***Pietro Binel***, *Marco Mazzotti*
10:09 Paper 568g: Crystallization Modeling of a Pharmaceutical Compound for Digital Twin Based in-Silico Optimization with Experimental Validation — ***Ayse Eren***, *Botond Szilagyi, Justin Quon, Charles D. Papageorgiou, Zoltan Nagy*

(569) Drug Delivery for Infectious Diseases

Thursday, Nov 11, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 108

Angela Brown, Co-Chair
Pedro Gonzalez-Cruz, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

8:00: Break
8:18: Break
8:36 Paper 569c: A Toxin-Triggered Vehicle for Targeted Delivery of Antibiotics— *Ziang Li,* ***Angela Brown***
8:54 Paper 569d: Anthrax Vaccine Development Using Pollen Shell-Based Mucosal Delivery System — ***Pedro Gonzalez-Cruz***, *Md Jasim Uddin, Harvinder Gill*
9:12 Paper 569e: Self-Assembling Prodrugs As Effective Antiretroviral Therapeutics — ***Han Wang***, *Maya Monroe, Charles Flexner, Honggang Cui*
9:30 Paper 569f: Design of an Antimicrobial Prodrug Against Multidrug-Resistant Bacteria — ***Meghan O'Leary***, *Sabrina Chen, Lars Westblade, Christopher Alabi*
9:48 Paper 569g: Microbe-Responsive and Microbe-Targeted Biomaterials for Drug Delivery (Invited Speaker) — ***Anita Shukla***

(570) Environmental and Automotive Catalysis I: Passive NOx Adsorber and NOx Reduction

Thursday, Nov 11, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 203

Eleni Kyriakidou, Chair
Arthur Shih, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

8:00 Paper 570a: Characterizing Rh Particles and Single-Atoms Supported on γ-Al_2O_3 for NO Reduction Using Probe-Molecule IR Spectroscopy and DFT— ***Alexander Hoffman***, *Chithra Asokan, Ibrahim Alfayez, Steven V. Nystrom Jr., Pavlo Kravchenko, Andrew (Bean) Getsoian, Phillip Christopher, David Hibbitts*
8:18 Paper 570b: Pt-CeO_2-Al_2O_3 Nanosheet Catalysts with Enhanced Lean/Rich Hydrothermal Aging Stability for Twc Applications — ***Junjie Chen***, *Chih-Han Liu, Todd Toops, Zhenglong Li, Eleni Kyriakidou*
8:36 Paper 570c: Effects of $C_{12}H_{26}$ and O_2 on NO Uptake on Pd/SSZ-13: Experiments and Modeling — ***Michael Harold***, *Mugdha Ambast*
8:54 Paper 570d: Mechanistic Aspects of Passive NO_x Adsorption on Pd-SSZ-13: Microkinetic Modeling to Explore the Role of Monomeric and Dimeric Sites— ***Bhuiyan Md. Rahman***, *Mugdha Ambast, Michael Harold, Lars Grabow*
9:12 Paper 570e: Effect of Cobalt Incorporation on the Stability of Ionic Pd in the Presence of Carbon Monoxide over Pd/BEA Passive NOx Adsorbers — *Jungkuk Lee,* ***Junjie Chen***, *Kevin Giewont, Pranaw Kunal, Todd Toops, Eric Walker, Eleni Kyriakidou*
9:30 Paper 570f: Bimetallic PdCu/SSZ-13 As Highly Efficient Passive NOx Adsorbers Under Industrially Relevant Feed Conditions — ***Pranaw Kunal***, *Todd Toops*
9:48 Paper 570g: Influence of Zcuoh, Z_2cu, and Extraframework Cu_xO_y Species in Cu-SSZ-13 on N_2o Formation during the Selective Catalytic Reduction of $NO_x$with NH_3 — ***Arthur J. Shih***, *Juan M. González, Ishant Khurana, Lucía Pérez Ramírez, Andres Peña L., Ashok Kumar, Aída Luz Villa*
10:06 Paper 570h: How Cu-SSZ-13 NH_3 Selective Catalytic Reduction Catalyst's Oxidation Activity Impacts on the Extent of Sulfur Poisoning — ***Yu-Ren Chen***, *Ashok Kumar, Di Wang, William Epling*

(571) Experimental Methods in Adsorption

Wednesday, Nov 10, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 308

Fateme Rezaei, Chair
Joeri Denayer, Co-Chair

Sponsored by: Adsorption and Ion Exchange

3:30 Paper 571a: New Pressure Drop Correlation for Structured Adsorbents with Parallel Triangular Channels — ***Ryan Sanders***, *Nima Mohammadi, Armin Ebner, James A. Ritter, Charles E. Holland*
3:48 Paper 571c: A New Theory for Adsorbate Specific Volumes and Saturation Loadings on 4A, 5A and 13X Zeolites — ***Kevin Loughlin***, *Dana Abouelnasr*
4:06 Paper 571d: Adsorption and Desorption of a Mixture of Volatile Organic Compounds: The Impact of Activated Carbon Porosity — ***Masoud Jahandar Lashaki***, *Samineh Kamravaei, Zaher Hashisho, John H. Phillips, James E. Anderson, Mark Nichols*
4:24 Paper 571e: Accurate High Pressure CH_4 Equilibrium Isotherms on NaY Using Adva and Xemis Apparatuses — *Riccardo Rea, Darren P. Broom, Matthew Gee, Mike Benham, Stefano Brandani,* ***Enzo Mangano***
4:42 Paper 571f: Measurements of Binary Adsorption Isotherms on Ammonium ZSM-5 Zeolite — ***Huong Giang Nguyen***, *Roger D. van Zee*
5:00 Paper 571g: Investigation of Departures from Ideal Adsorption Behavior by Binary Gas Mixtures on Metal-Organic Framework Adsorbents — ***Danny Shade***, *Bartosz Marszalek, Krista Walton, David Sholl*
5:18 Paper 366c: Combining Novel Methodologies Based on NMR Relaxometry and Gas Adsorption for Reliable Surface Assessment of Nanoporous Materials— ***Carola Schlumberger***, *Matthias Thommes*
5:36 Paper 101a: Enhancing the Hydrolytic Stability of Porous Boron Nitride for Use in Industrial Molecular Separations — ***Anouk L'hermitte***, *Daniel M. Dawson, Pilar Ferrer, Kanak Roy, Takuya Hirosawa, Georg Held, Tian Tian, Toshihiro Isobe, Sharon E. Ashbrook, Camille Petit*

(572) Formulation for Drug Delivery

Thursday, Nov 11, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 101

Brendon Ricart, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

8:00 Paper 572a: Thermoplastic Copolyesters: A Novel Solution for 3D-Printed, Implantable Drug Delivery Devices — ***Ioannis Koutsamanis***, *Amrit Paudel, Carolina Alva, Laura Wiltschko, Martin Spörk*
8:24 Paper 572c: Investigation of Carrier Type and Blending Parameters on the Performance of a Dual-Combination DPI: A Comparative *in-Vitro-in-Silico* Study— ***Michela Beretta***, ***Snezana Radivojev***, *Valerie Reinisch, Viktoria Rehbein, Joana Pinto, Eleonore Fröhlich, Amrit Paudel*
8:48 Paper 572e: Nanoemulsion-Loaded Capsules for Controlled Delivery of Lipophilic Active Ingredients — ***Liang-Hsun Chen***, *Li-Chiun Cheng, Patrick S. Doyle*
9:12 Paper 572f: Transport- and Reaction-Modeling of Nanocarriers for Cancer Therapeutics Via Experimental and *in-Silico* approaches — ***Omkar Bhatavdekar***, *Mihalis Kavousanakis, Domenico Bullara, Stavroula Sofou, Ioannis G. Kevrekidis*
9:36 Paper 103a: Spray-Dried Lipid-Microparticles for Inhalation: Correlation between Solid State and Processability — ***Carolina Corzo***, *Agnes Fuchsbichler, Dirk Lochmann, Sebastian Reyer, Andreas Zimmer, Sharareh Salar-Behzadi*
10:00 Paper 103b: Acid-Responsive Colloidal Drug Aggregates Escape from the Endolysosomal Pathway — ***Eric Donders***, *Kai Slaughter, Christian Dank, Ahil Ganesh, Brian Shoichet, Mark Lautens, Molly S. Shoichet*

(573) Fundamentals and Applications for Municipal Solid Waste Treatment and Valorization

Thursday, Nov 11, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 309

Matthew Alexander, Chair
Enoch Nagelli, Co-Chair
Robert Peters, Co-Chair
Mohamed Mostafa, Co-Chair

Sponsored by: Solid and Hazardous Waste

8:00 Paper 573a: Analysis of Plastic-Derived Fuel Oil Produced from Plastic Waste Via Slow Pyrolysis Operations — ***Chandni Joshi***, *Jeffrey Seay, Kevin Miller*
8:20 Paper 573b: Civic Environmentalism and Waste Recycling: The Role of Community Social Capital in Promoting Eco-Friendly Behaviors — ***Robert Peters***, *Gail Wallace*
8:40 Paper 573d: Automatic Anaerobic Digestion Microplant for Decentralised Management of Waste — ***Ernesto Hernandez***
9:00 Paper 573e: Anaerobic Digestion of Different Type of Wastepaper and Cardboard: Effect of Enzymatic Pretreatment — ***Fokion Kaldis***, *Ioannis Stamou, Ioannis Zarkadas, Dimosthenis Sarigiannis*

(574) Fundamentals of Catalysis and Surface Science II: Metals

Thursday, Nov 11, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 207

Shu Hu, Chair
Andrew R Teixeira, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

8:00 Paper 574a: Citral Hydrogenation over Nipt and Cupt Dilute Alloy Catalysts— ***Madelyn R. Ball***, *Iman Nezam, Dong-Chan Lee, Faisal M. Alamgir, Christopher W. Jones*
8:18 Paper 574b: Kinetics of Ethylene Epoxidation and Chlorine Moderation over Promoted silver catalysts — ***Krishna Iyer***, *Aditya Bhan, James W. Harris*
8:36 Paper 574c: Computational and Experimental Insights into Reactive Forms of Oxygen Species on Dynamic Ag Surfaces Under Ethylene Epoxidation Conditions — *Changming Liu, Devinda P. Wijewardena,* ***Anna Sviripa***, *David Flaherty, Christopher Paolucci*
8:54 Paper 574e: Mechanistic Details of Vinyl Acetate Synthesis on Pd/SiO_2 — *Zhaoru Zha, Georgios Giannakakis,* ***Prashant Deshlahra***
9:12 Paper 574f: Kinetic Analysis of CO Methanation on Sn Promoted Pt/γ-Al_2O_3 Catalysts — ***Robson Schuarca***, *Jesse Bond*
9:30 Paper 574g: Methane Activation over Transition Metal Single Atom Doped (211) Facets of Pt and Pd — ***Debtanu Maiti***, *Michael Harold, Lars Grabow*
9:48 Paper 574h: Enantioselective Reaction Kinetics of Tartaric Acid on Surfaces Vicinal to Cu(111) — ***Carlos Fernandez-Caban***, *Andrew J. Gellman*

(575) Immunotherapy

Thursday, Nov 11, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 109

Ashish Kulkarni, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

8:00: Break
8:18 Paper 575h: Engineering Polymeric Nanoparticles to Probe Innate Immunity — ***Ashish Kulkarni***
8:54 Paper 575b: Granzyme B Nanoreporter for Early Monitoring of Tumor Response to PD-L1 Checkpoint Blockade — ***Anh Nguyen***, *Anujan Ramesh, Sahana Kumar, Dipika Nandi, Anthony Brouillard, Alexandria Wells, Leonid Pobezinsky, Barbara Osborne, Ashish Kulkarni*
9:12 Paper 575c: Electrostatic-Driven Interactions Enhance Intratumoral Retention, Distribution, and Antitumor Efficacy of Immune Checkpoint Blockade Antibodies — ***Rashmi Mohanty***, *Mae M. Lewis, Esther Y. Maier, Melissa Soto, Debadyuti Ghosh*
9:30 Paper 575e: Real-Time Imaging of Macrophage Immunotherapy Using a Novel Nitric Oxide Nanoreporter — ***Anujan Ramesh***, *Sahana Kumar, Anthony Brouillard, Dipika Nandi, Ashish Kulkarni*
9:48 Paper 575g: Engineering Injectable Polymeric Cryogels for Biomedical Applications: From Tissue Engineering to Immunotherapy (Invited Speaker)— ***Sidi A Bencherif***

(576) In Honor of the 2018 William H. Walker Award Winner I (Invited Talks)

Thursday, Nov 11, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 210

David Flaherty, Chair
Justin Notestein, Co-Chair
Rajamani Gounder, Co-Chair
Aditya Bhan, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

8:00 Paper 576a: Opportunities for Responsibly Realizing the Potential of Shale Gas Resources — ***Fabio H. Ribeiro***
8:20 Paper 576b: Mesocatalysis: An Investigation on the Complexity of Catalysis — ***Weiping Ding***
8:40 Paper 576c: Oxidative Dehydrogenation As a Platform for Fundamental Studies in Supported Oxides and a Playground for Tandem Catalysis — ***Justin Notestein***
9:00 Paper 576d: Combining DFT and Kinetic Monte Carlo Simulations to Model Reactions and Transport in MFI Zeolites over Large Time and Length Scales — *Mykela DeLuca, **David Hibbitts***
9:20 Paper 576e: Deciphering Mechanisms of Reaction and Deactivation over Isostructural Metal-Organic Frameworks for Small-Molecule Oxidation — *Rachel A. Yang, **Michele Sarazen***
9:40 Paper 576f: Dioxygen Activation Pathways in Mars-Van Krevelen Redox Cycles — ***Stephanie Kwon**, Prashant Deshlahra, Enrique Iglesia*
10:00 Paper 576g: Catalysis within Slippery Solvents in Small Spaces — ***David Flaherty**, Daniel Bregante, Matthew Chan, E. Zeynep Ayla, Diwakar Shukla*

(577) Lithium and Beyond: Fundamental Advances in High Performance Batteries I

Thursday, Nov 11, 8:00 AM
Sheraton Back Bay, Commonwealth

Joshua Gallaway, Chair
Shuya Wei, Co-Chair
Alexander Urban, Co-Chair
Nian Liu, Co-Chair

Sponsored by: Electrochemical Fundamentals

8:00: Break
8:15 Paper 577a: Bioinspired Nanoporous Ion Conducting Membranes for Next Generation Batteries — ***Ahmet Emre**, Emine Sumeyra Turali-Emre, Jinchen Fan, Nicholas Kotov*
8:30 Paper 577c: Tailored Trilayer Separator for Extreme Temperature Lithium-Sulfur Batteries — ***Mihit Parekh**, Manikandan Palanisamy, Vilas G. Pol*
8:45 Paper 577d: Dual Pseudocapacitive Oxides Accelerate Kinetics of Sulfur Intermediates in Lithium-Sulfur Batteries — ***Fang Liu**, Geng Sun, Bruce Dunn, Philippe Sautet, Yunfeng Lu*
9:00 Paper 577e: Molecular-Level Characterization of the Electrode-Electrolyte Interfaces in Li Batteries — ***Lauren Marbella***
9:20 Paper 577f: Detecting the Onset of Li Plating during Fast Charging of Li-Ion Batteries Using *Operando E*lectrochemical Impedance Spectroscopy— ***David Brown**, Eric McShane, Zachary Konz, Kristian Knudsen, Bryan McCloskey*
9:35 Paper 577g: Catalyst Design for Metal Air Batteries Utilizing a Four-Electron Oxidation and Reduction of Metal Oxides — ***Jaclyn Lunger**, Michal Bajdich, Yang Shao-Horn*
9:50 Paper 577h: Solvation Effects on Lithium Ion Transport and Reaction on Lithium Metal Anodes — ***Stefany Angarita-Gomez**, Perla B. Balbuena*

(578) Membrane Formation

Thursday, Nov 11, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 301

Ngoc Bui, Co-Chair
Katie Dongmei Li-Oakey, Co-Chair

Sponsored by: Membrane-Based Separations

8:00 Paper 578a: Atomistic Simulations of Aromatic Polyamide Membrane— ***Tao Wei***
8:15: Break
8:30 Paper 578d: Designing Thin–Film Composite Membranes Based on Amorphous Poly(ethylene oxide) for CO_2/Gas Separation — ***Gengyi Zhang**, Thien Tran, Haiqing Lin*
8:45 Paper 578e: Highly Permeable Matrimid Substrates with Bicontinuous Structure for a CO_2-Selective Composite Membrane — ***Ruizhi Pang**, Kai Chen, Yang Han, Yutong Yang, W.S. Winston Ho*
9:00 Paper 578g: Antimicrobial Membrane Filters for Face Mask Production— ***Ebuka Ogbuoji**, Isabel Escobar*
9:15 Paper 408f: Prospects for Controllable Ultrathin Membrane Synthesis Using Molecular Layer Deposition — ***David Bergsman***
9:30 Paper 607f: Reformulation of the Solution-Diffusion Theory of Organic Solvent Nanofiltration and Reverse Osmosis: Effect of Sorption, Diffusion, Pressure and Molecular Interactions — *Kelly Bye, **Michele Galizia***

(579) Membranes for CO_2 Capture

Thursday, Nov 11, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 306

Yang Han, Co-Chair
Junyi Liu, Co-Chair

Sponsored by: Membrane-Based Separations

8:00 Paper 579a: A Polystyrene Sulfonate Assisted Polyethylenimine Membrane for Stable, Scalable and Highly Effective CO_2/N_2 Separation— ***Huanghe Li**, Shenxiang Zhang, Miao Yu*
8:25 Paper 579b: Sorption-Enhanced Mixed-Gas Transport in Amine Functionalized Polymers of Intrinsic Microporosity (PIMs) — ***Katherine Mizrahi Rodriguez**, Francesco Maria Benedetti, Naksha Roy, Albert X. Wu, Zachary Smith*
8:50 Paper 579c: Tuning Ether Motifs in Polymers Membranes for CO_2/N_2Separation — ***Yasemin Basdogan**, Zhen-Gang Wang*
9:15 Paper 579e: In Situ Growth of ZIFs in Polybenzimidazole to Achieve Superior H_2/CO_2 Separation Performance — ***Leiqing Hu**, Vinh Bui, Haiqing Lin*
9:40 Paper 579f: Upscaling of Facilitated Transport Membranes for Hydrogen Purification from Coal-Derived Syngas — ***Yang Han**, Yutong Yang, Ruizhi Pang, Winston Ho*
10:05 Paper 579d: Pushing the Limit of Å-Scale Nanopore Engineering for Carbon Capture from Graphene Membrane — ***Kuang Jung Hsu**, Kumar Varoon Agrawal*

(580) Microporous and Mesoporous Materials I: Synthesis-Structure-Function Relations

Thursday, Nov 11, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 208

Viktor Cybulskis, Chair
Praveen Bollini, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

8:00 Paper 580a: Smaller, Faster, Better: Distinguishing the Timescales of Finned Zeolites Via Time-Resolved Amine Titration — ***Choongsze Lee**, Heng Dai, M. Alexander Ardagh, Jeffrey Rimer, Michael Tsapatsis, Paul Dauenhauer*
8:18 Paper 580b: Impact of Microporosity on the Catalytic Performance of Micro-Mesoporous Aminosilica Materials for the Knoevenagel Condensation— ***Ashwin Kane**, Nicholas Brunelli*
8:36 Paper 580c: Characterization and Analysis of Ring Topology of Zeolite Frameworks — ***Jerry Crum**, Justin Crum, William Schneider*
8:54 Paper 580d: Investigation of Crystallization of Siliceous LTA Zeolite Using Raman Spectra — ***Song Luo**, Tongkun Wang, Long Qi, Geoffrey Tompsett, Michael T. Timko, Scott M. Auerbach, Wei Fan*
9:12 Paper 580e: Quantitative Connections between Copper Site Proximity and Binuclear Active Sites for Partial Methane Oxidation to Methanol in Cu-CHA Zeolites — ***Laura Wilcox**, Yujia Wang, William Schneider, Rajamani Gounder*
9:30 Paper 580f: Low Temperature Pd Mobility in Ion-Exchanged Zeolite Hydrocarbon Traps — ***Ryan Zelinsky**, William Epling*
9:48 Paper 580g: Distributions of Al Atoms in Chabazite Zeolite Frameworks and Their Effects on Catalytic Reaction Properties — ***Michael Schmithorst**, Zachariah Berkson, Subramanian Prasad, Bradley F. Chmelka*
10:06 Paper 580h: Tailoring the Physicochemical Properties and Performance of FAU Catalysts with Heteroatoms — ***Adam J. Mallette**, Deependra Parmar, Sungil Hong, Emily Freeman, Sarah A. Saslow, Sebastian Mergelsberg, Radha Kishan Motkuri, James Neeway, Giannis Mpourmpakis, Jeffrey Rimer*

(581) Modeling of Lipid Membranes and Membrane Proteins

Thursday, Nov 11, 8:00 AM
Marriott Copley Place, Salon H/I

Reid Van Lehn, Chair
Diwakar Shukla, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

8:00 Paper 581a: Elucidating Mechanisms of Substrate Transport in Neurotransmitter Transporters — ***Diwakar Shukla***
8:15 Paper 581b: Mechanism of Selective Ion Transport through Kidney Tight Junctions — ***Jingjing Ji**, Nandhini Rajagopal, Shikha Nangia*
8:30 Paper 581c: Simulation Study of the Long-Periodicity Phase of the Stratum Corneum — ***Parashara Shamaprasad**, Christopher Iacovella, Annette Bunge, Clare McCabe*
8:45 Paper 581d: Computational Study of Lipid Dynamics within a Complex Realistic *Staphylococcus Aureus* Membrane with Lipid and Leaflet Diversity— ***Faramarz Joodaki**, Lenore M. Martin, Michael Greenfield*
9:00 Paper 581e: Leaflet Asymmetry in Biological Lipid Membranes — ***Nelly Raissa Setchie-Tchato**, Faris Amer, Patrick Marsch, Nathena Murray, Isabelle Tawyer, Yinghui Dai, Allyson Karmazyn, Nandhini Rajagopal, Shikha Nangia*
9:15 Paper 581f: Electromechanics of Lipid Bilayers: A Dimensionally Reduced Theory — ***Yannick Azhri Din Omar**, Zachary Lipel, Kranthi K. Mandadapu*

(582) Molecular and Data Science Modeling of Adsorption I

Monday, Nov 8, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 110

Li-Chiang Lin, Chair
Gennady Gor, Co-Chair
Alina Emelianova, Co-Chair

Sponsored by: Adsorption and Ion Exchange

3:30 Paper 582a: Accelerated Discovery of Metal-Organic Frameworks for Gas Separations Using Bayesian Optimization — ***Eric Taw**, Jeffrey B. Neaton*
3:45 Paper 582b: Water-Bridges Substitute for Defects in Amine-Functionalized Uio-66, Boosting CO_2 Adsorption — *Arianjel Hernandez, Rebekah K. Impastato, Mohammad I. Hossain, **Brooks Rabideau**, Thomas Glover*
4:00 Paper 582d: Smallest Repeating Units: A New Descriptor for Representing Zeolites and Periodic Frameworks — ***Akhilesh Gandhi**, M M Faruque Hasan*
4:15 Paper 582g: Incorporating Flexibility Effects into Metal-Organic Frameworks Adsorption Simulations — ***Zhenzi Yu**, Dylan Anstine, Salah Eddine Boulfelfel, Coray M. Colina, David Sholl*
4:30 Paper 582h: Revealing Specifics of Gas Adsorption in Metal-Organic Frameworks from Compartmentalization of Adsorption Isotherms — ***Shivam Parashar**, Skandan Venkatraman, F. Silvio P. Dantas, Alexander Neimark*
4:45 Paper 582i: Deep Learning Combined with IAST to Screen Thermodynamically Feasible MOFs for

Adsorption-Based Separation of Multiple Binary Mixtures — *Ryther Anderson, **Diego Gomez Gualdron***
5:00 Paper 582j: Computational Screening to Identify Metal-Organic Frameworks for Water Harvesting — ***Faramarz Joodaki**, Andrew Rosen, Brandon C. Bukowski, Haoyuan Chen, Randall Snurr*
5:15 Paper 412g: Molecular Dynamics Simulations of Enantiomeric Separations As an Interfacial Process in HPLC — *Cynthia J. Jameson, **Xiaoyu Wang**, Sohail Murad*

(583) Multi-Scale Modeling

Thursday, Nov 11, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 206

Anthony Dixon, Chair
Sankar Dinesh Kumar Kalaga, Co-Chair
Andrew Adamczyk, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

8:00 Paper 583a: Evaluation of Multi-Scale Models for Ethylene Epoxidation in a Fixed Bed Reactor — ***Anthony Dixon***
8:18 Paper 583b: Combining Ab Initio and Classical Molecular Dynamics Simulations to Predict the Implication of Charged Osdas on of Al Siting Preferences in CHA. — ***Xiaoyu Wang**, Yujia Wang, Edward J. Maginn, William Schneider*
8:36: Break
8:54 Paper 583e: First-Principles-Informed Kinetic Modelling in Operando Catalysis Studies: CO Oxidation on Metal Nanoparticles — ***Astrid Boje**, Henrik Ström, Anders Hellman*

(584) Pharma 4.0 (Advanced Controls, Process Automation, Data Analytics, etc.) in Drug Substance and Drug Product

Thursday, Nov 11, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 102

Sudarshan Ganesh, Chair
Dominique Hebrault, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

8:00 Paper 584a: Process Modeling and Control of Digital Biopharmaceutical Manufacturing — ***Moo Sun Hong**, Richard Braatz*
8:24: Break
8:48 Paper 584c: The Use of Hybrid Modeling Schemes in the Development of a Probabilistic Condition Monitoring System for a Continuous Drug Product Manufacturing Process — ***Rexonni Lagare**, M.Ziyan Sheriff, Zoltan Nagy, Gintaras V. Reklaitis*
9:12 Paper 584d: Identifying Potential One-Pot Synthesis from Computer-Planned Synthetic Routes — ***Hanyu Gao**, Klavs Jensen*
9:36 Paper 584e: Optimizing Energy Efficiency of a Twin Screw Granulation Process Using a Physics-Constrained Hybrid Model — ***Chaitanya Sampat**, Rohit Ramachandran*
10:00 Paper 584f: Optimization and Control of Modular Chemical Systems for Continuous Manufacturing — ***Anastasia Nikolakopoulou**, Richard D. Braatz*

(585) Polymer Simulations 2: Structure and Fundamentals

Thursday, Nov 11, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 209

Janani Sampath, Chair
Poornima Padmanabhan, Co-Chair

Sponsored by: Polymers

8:00 Paper 585a: Insights from Molecular Dynamics Simulation into the Dynamics and Glass Formation Behavior of Polymers Near Interfaces and Under Nanoconfinement — ***David Simmons***
8:30 Paper 585b: Entanglements and Chain Conformations in Model Polymer-Grafted Nanoparticle Monolayers — ***Nicholas Liesen**, Lisa Hall*
8:44 Paper 585c: High-Throughput Initialization and Simulation of Thermoplastic Fusion Bonding — ***Chris Jones**, Rainier Barrett, Jenny Fothergill, Eric Jankowski*
8:58 Paper 585d: Computational Studies of Order-Disorder Transition in Block Copolymer Topological Blends — ***Rahul Kumar**, Amy D. Goodson, Oluwafemi Alli, Clayton Chamness, Isabella Miserocchi, Julie Albert, Henry Ashbaugh*
9:12 Paper 585e: Comparison of Friction Parameterization from Dynamics and Material Properties for a Coarse-Grained Polymer Melt — ***Lilian Johnson**, Frederick Phelan Jr.*
9:26 Paper 585f: Effect of Reaction Kinetics on Mechanical and Rheological Properties of Vitrimers — ***Alessandro Perego**, Fardin Khabaz*
9:40 Paper 585h: Geometry of Stable Spherical Phases in Diblock Copolymer Melts — ***Ryan Collanton**, Kevin Dorfman*
9:54 Paper 585i: Using Reactive Dissipative Particle Dynamics to Understand Local Shape Manipulation of Polymer Vesicles — ***Douglas Tree**, Qinyu Zhu*
10:08: Break
10:22 Paper 723e: Altering PLGA-Peg, PLGA and Peg Oligomer Extension to Understand Driving Forces behind Protein/Polymer Binding, Using Atomistic Molecular Dynamics. — ***Christopher Nyambura**, Jim Pfaendtner, Elizabeth Nance*

(586) Process Intensification through Process Systems Engineering

Thursday, Nov 11, 8:00 AM
Sheraton Back Bay, Back Bay Ballroom C

Davood Babaei Pourkargar, Co-Chair
Maria Papathanasiou, Co-Chair

Sponsored by: Systems and Process Design

8:00 Paper 586a: Superstructure Optimization Enabled Design Heuristics and Material Property Targets for Continuous Diafiltration Membrane Cascades— ***Elvis Eugene**, Noah Wamble, William Phillip, Alexander Dowling*
8:21 Paper 586b: Optimal Integration of Process Design and Dynamic Transitions for Catalytic Distillation Columns: A Discrete-Steepest Descent Framework — *David A. Linan, **Luis Ricardez-Sandoval***
8:42 Paper 586c: Novel Module-Based Design and Optimization Approach for Intensified Membrane Reactor Systems — ***Brent Bishop**, Fernando V. Lima*
9:03 Paper 586d: Techno-Economic Analysis of a Dynamic Packed Reactive Distillation Column for Renewable Biosurfactant Production — ***Khalid Rashid**, Christoph Krumm, Trenton Wilke, Babatunde A. Ogunnaike*
9:24 Paper 586e: Intensified Process Design Alternatives for the Diethyl and Ethyl-Methyl Carbonate Production — *Gloria Azucena Buitimea-Cerón, Nancy Medina-Herrera, **Salvador Tututi-Avila***
9:45 Paper 586f: A Process Intensification Synthesis Framework for the Design of Divided Wall Columns — ***Yuhe Tian**, Vaishnav Meduri, Rahul Bindlish, Efstratios N. Pistikopoulos*
10:06 Paper 586g: Optimization Modeling for Advanced Syngas to Olefin Reactive Systems Under Parameter Uncertainty — ***Can Ekici**, Christopher R. Ho, Joseph DeWilde, Paul Witt, Lorenz Biegler*

(588) Recent Advances in Molecular Simulation Methods

Thursday, Nov 11, 8:00 AM
Marriott Copley Place, Salon J/K

Harish Vashisth, Chair
Diego Gomez Gualdron, Co-Chair
Mona Minkara, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

8:00 Paper 588a: Efficient Measurement of Anharmonic Mechanical Properties of Crystals Using Normal-Mode Mapping — ***Sabry G. Moustafa**, Andrew Schultz, David Kofke*
8:15 Paper 588b: Diabat Method for Polymorph Free Energies — ***Kartik Kamat**, Baron Peters*
8:30 Paper 588c: How to Quantify and Avoid Finite Size Effects in Computational Studies of Crystal Nucleation — ***Sarwar Hussain**, Amir Haji-Akbari*
8:45 Paper 588e: Improved Configurational Sampling By the the Introduction of Alchemical Variable in Metadynamics — ***Wei-Tse Hsu**, Pascal Merz, Giovanni Bussi, Michael Shirts*
9:00 Paper 588g: Configurational-Bias Monte Carlo Simulation to Predict the Supramolecular Self-Assemblies of Amphiphiles — ***Silabrata Pahari**, Mustafa Akbulut, Joseph Kwon*
9:15 Paper 588h: Bypassing Backmapping By Learning the Noise of Electronically Coarse-Grained Models — ***Nicholas Jackson***
9:30 Paper 588i: Exploration of the Secondary Structure Peptoid Folding Landscape with Metadynamics — ***Sarah Alamdari**, Kaylyn Torkelson, Selina (Xiaoqian) Wang, Jim Pfaendtner*

(589) Solid-Liquid Interfaces

Thursday, Nov 11, 8:00 AM
Sheraton Back Bay, Back Bay Ballroom A

Stephen Martin, Chair
Younjin Min, Co-Chair
Laura Mears, Co-Chair
Siamak Nejati, Co-Chair

Sponsored by: Interfacial Phenomena

8:00 Paper 589a: Novel Highly Fluorinated Ionic Liquids As Nanometer-Thick Media Lubricants — ***Bingchen Wang**, Alan Tirado, Catherine Moran, Lei Li*
8:15 Paper 589c: Fate of Fluids in, on, and between Phobic Fiber Networks— ***Sumner Dudick**, Dennis Hess, Victor Breedveld*
8:30 Paper 589d: Controlling Membrane Flux By Changing the Contact Angle of Liquids — ***Dongjin Seo**, Daniel Lippert, Jacob Burnham, Diako Mahmodi, Seokjhin Kim*
8:45 Paper 589g: Interfacial and Cohesive Properties of Ocular Epithelia— ***Chunzi Liu**, Gerald Fuller*
9:00 Paper 589h: Cooperative Hydrogen Bonding – Towards Robust Underwater Adhesion — ***Joelle Frechette**, Zachary Lamberty, Ngon Tran, Daniel B. Knorr Jr.*
9:15 Paper 589j: Effect of Surface Wettability on Interfacial Adhesion of Thermosetting Polymer Composites — ***Ye Wang**, Antoine P. Delarue, Christopher J. Hansen, Amy M. Peterson*
9:30 Paper 135d: Study of MF Membranes for Microalgae Dewatering and Surface Modification for Fouling Mitigation — ***Erda Deng**, Xiaoyi Chen, Darius Rub, Xiaoci Lin, Haiqing Lin*
9:45 Paper 135c: The Effect of Mechanical Property of Nanostructured Polymer Thin Films on the Surface Tension-Driven Bactericidal Efficacy — ***Ruwen Tan**, Nicolas Marzolini, Thomas Angelini, Kwangcheol C. Jeong, Yeongseon Jang*
10:00 Paper 135a: Surface Wettability and Roughness Play a Key Role in Bacterial Adsorption Kinetics — ***William DeFlorio**, Jun Kyun Oh, Shuhao Liu, Li Hao, Sang Bum Kim, Younjin Min, Matthew Taylor, Alejandro Castillo, Luis Cisneros-Zevallos, Mustafa Akbulut*

(590) Synthetic Biology: Microbiome Engineering

Thursday, Nov 11, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 110

Nathan Crook, Chair
Eric Young, Co-Chair

Sponsored by: Bioengineering

8:00 Paper 590a: Engineering Multilevel CRISPR-Based Kill-Switches for Probiotic *Escherichia coli* — ***Austin Rottinghaus***, *Aura Ferreiro, Gautam Dantas, Tae Seok Moon*
8:18 Paper 590b: Programming Gene Expression in Multicellular Organisms for Physiology Modulation through Engineered Bacteria — ***Baizhen Gao***, *Qing Sun*
8:36 Paper 590c: Fungal Highways Enable Migration and Communication of Engineered Bacteria in Soil — *Nilesh K Sharma, Andres F Carrillo, Jaclyn Thompson, Natalie Farny,* ***Eric Young***
8:54 Paper 590d: Multiplexed Information Flow Via H_2O_2-Facilitated Electrogenetic CRISPR for Enabling "Multilingual" Communication Among Biological Networks — ***Sally Wang***, *Eric VanArsdale, Chen-Yu Tsao, Jinyang Li, William Bentley*
9:12 Paper 590e: Programming Multicellular Genetic Circuits and Sequential Logic in Synthetic Microbial Consortia — ***Min Zeng***, *Brian Voke, Lauren B. Andrews*
9:30 Paper 590f: Chassis Engineering for Heterologous Protein Production in *E. coli* Nissle 1917 — *Halimatun Zainuddin,* ***Thomas J. Mansell***
9:48 Paper 590g: From Cattle to Humans: Probing the Respiratory Microbiome— ***Mohit Verma***

(591) Systems and Quantitative Biology: Metabolic Modeling

Thursday, Nov 11, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 111

Christopher Kieslich, Chair
Benjamin Woolston, Co-Chair

Sponsored by: Bioengineering

8:00 Paper 591a: Towards Cybernetic Modeling of Biological Processes in Mammalian Systems—Lipid Metabolism in the Murine Macrophage — ***Lina Aboulmouna***, *Rubesh Raja, Sana Khanum, Shakti Gupta, Mano Maurya, Shankar Subramaniam, Doraiswami Ramkrishna*
8:18 Paper 591b: Omics-Informed Metabolic Modeling Identifies Regulatory Mechanisms in *Staphylococcus Aureus* mutants — ***Mohammad Mazharul Islam***, *Vinai Chittezham Thomas, Rajib Saha*
8:36 Paper 591c: Dynamic Genome-Scale Metabolic Modeling Suggests the Establishment of Mutualism without Co-Evolution within a Synthetic Microbiome— ***Kiumars Badr***, *Q. Peter He, Jin Wang*
8:54 Paper 591d: Modeling Metabolic Networks Using Graph Neural Networks— ***Shekhar Mishra***, *Ziyu Wang, Huimin Zhao*
9:12 Paper 591e: Using Genome-Scale Metabolic Models and Machine Learning to Design Condition-Specific Combination Therapies — ***Carolina Chung***, *Harkirat Singh Arora, Sriram Chandrasekaran*
9:30 Paper 591f: Modeling Inflammatory Lipid Dynamics Using a Cybernetic Framework and Information-Theoretic Approaches — ***Sana Khanum***, *Lina Aboulmouna, Rubesh Raja, Mohsen Heidari Khoozani, Mano Maurya, Shakti Gupta, Shankar Subramaniam, Doraiswami Ramkrishna*
9:48 Paper 591g: Introducing New Approaches to Gapfilling and Dynamic Flux Balances Analysis for Genome-Scale Models — ***Rajib Saha***

(592) Thermochemical Conversion of Biomass

Thursday, Nov 11, 8:00 AM
Marriott Copley Place, Suffolk

Justinus Satrio, Chair
Sunkyu Park, Co-Chair

Sponsored by: Forest and Plant Bioproducts Division

8:00 Paper 592a: Integrated Biochemical and Hydrothermal Processing of Corn Stover for Fuels and High Value Products — ***Bharathkiran Maddipudi***, *Vinod S. Amar, Khang Huynh, Anuj Thakkar, Katelyn Shell, Runzhou Huang, Anuradha Shende, Sergio Hernandez, Sandeep Kumar, Ram Gupta, Hao Fong,* ***Rajesh Shende***, ***Bharathkiran Maddipudi***
8:15 Paper 592b: Synergistic Effects on Co-Hydrothermal Liquefaction of High Ash Corn Stover and Halogenated Plastic — ***Soudeh Banivaheb***, *Nepu Saha, Toufiq Reza*
8:30 Paper 592c: Catalytic Hydropyrolysis of Rice Husk over a Hierarchical Micro-Mesoporous Composite Catalyst — *Zhaoying Li, Zhaoping Zhong, Qirong Yang, Ting Liu, Wei Lv, Gabriel Viana Sueth Seufitelli,* ***Fernando Resende***
8:45 Paper 592d: Effect of Recycling Potassium Hydroxide on Surface Morphology Superactivated Hydrochar Derived from Loblolly Pine — ***Al Ibtida Sultana***, *Toufiq Reza*
9:00 Paper 592e: Implementing Autothermal Reactions in a Novel Fluidized Bed Model for Fast Pyrolysis Applications — ***Benjamin Caudle***, *Maximilian Gorensek, Chau-Chyun Chen*
9:15 Paper 592f: Double the Pleasures: Perennial Grasses As Soil Phytoremediation Agents and Renewable Carbon Resources for Fuels and Chemicals — *Maria Nydia Lynch,* ***Justinus Satrio***

(593) Thermodynamics at the Nanoscale

Thursday, Nov 11, 8:00 AM
Marriott Copley Place, Simmons

Nathan Mahynski, Chair
Sriramvignesh Mani, Co-Chair
Utkarsh Kapoor, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

8:00 Paper 593a: Free Energy Simulations Along Entropic Pathways: Sampling Phase Transitions at the Nanoscale — *Caroline Desgranges,* ***Jerome Delhommelle***
8:14 Paper 593b: Probing Metal Nanocrystal Shapes and Shape Transformations Using Replica Exchange Molecular Dynamics Simulations— ***Tianyu Yan***, *Kristen Fichthorn*
8:28: Discussion
8:54 Paper 593d: Free Energy Calculation on Human Beta Defensin Translocation through Bacterial Lipid Membranes — ***Ann Brewer***, ***Liqun Zhang***
9:08 Paper 593e: Phase Transition and Criticality of Methane Confined in Nanopores — ***Huan Yang***, *Xingdong Qiu, Morteza Dejam, Sugata P. Tan, Hertanto Adidharma*
9:22 Paper 593f: [Invited Talk] Re-Entrant Dynamics and Anomalous Fluctuations in Strongly Confined Liquids — ***Jeremy Palmer***
9:48 Paper 593g: Free Energy Landscape of Alkanes Confined within Supramolecular Complexes — ***Busayo Alagbe***, *Bruce C. Gibb, Henry Ashbaugh*
10:02 Paper 593h: Hydration Free Energies of Linear Alkanes Studied Via Molecular Simulations — ***Sumit Sharma***, *Himanshu Singh*
10:16 Paper 593i: Molecular Dynamics Simulations of Nanostructures Formed By Hydrophobins and Oil in Seawater — *Andres Vodopivec, Yuwu Chen, Paul Russo,* ***Francisco Hung***

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

Thursday, Nov 11, 12:30 PM
Marriott Copley Place, Salon J/K

Cory Simon, Chair
Kaihang Shi, Co-Chair
Yamil Colón, Co-Chair
Obioma Uche, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

12:30 Paper 594a: The Influence of Coverage on Entropy: Changes in Vibrational Frequencies of CO on Pt (111) — ***Jongyoon Bae***, *Andrew A. Peterson, C Franklin Goldsmith*
12:45: Break
1:00 Paper 594c: Dynamical Evolution of Atomically Dispersed Catalysts: Ab Initio Molecular Dynamics Analysis of Thermal and Adsorbate-Induced Metal Atom Migration — ***Nicholas Humphrey***, *Shaama Mallikarjun Sharada, Selin Bac*
1:15 Paper 594d: Uncovering a Universal Molecular Mechanism of Salt Ion Adsorption at Solid/Water Interfaces — ***Rahul Prasanna Misra***, *Daniel Blankschtein*
1:30 Paper 594g: Predicting the Equilibrium Adsorption Morphologies of Surfactant Molecules at Metal-Water Interfaces Via Advanced Molecular Dynamics Simulations — ***Himanshu Singh***, *Sumit Sharma*
1:45 Paper 594i: Understanding the Role of Charge Distribution and Pore Size for Water Vapor Adsorption in Idealized Nanoporous Materials — ***Krishnendu Mukherjee***, *Yamil Colón*
2:00 Paper 594j: Phase Behavior of Confined Multiple Sites Associating Lj Fluids in Functionalized Slit Pore: A Monte Carlo Study — ***Sashanka Sekhar Mandal***, *Sandip Khan*

(595) Biomaterial Scaffolds for Tissue Engineering I

Thursday, Nov 11, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 209

Gulden Camci-Unal, Chair
Mario Moisés Álvarez, Co-Chair
Samira Azarin, Co-Chair
Amol Janorkar, Co-Chair

Sponsored by: Biomaterials

12:30 Paper 595a: Self-Fitting, Shape Memory Polymer Scaffolds for Bone Defect Repair — ***Melissa Grunlan***
1:06 Paper 595b: Two-Phase Scaffolds with Nanoparticle Decorations for Growth Factor Delivery for Bone Regeneration — ***Mariya Shevchuk***, *Nicholas Peppas*
1:24: Break
1:42 Paper 595d: Granular Matrigel: Restructuring a Trusted Scaffolding Material to Improve Matrix Permeability — ***Zahra Mahdieh***, *Michelle D. Cherne, Jacob P. Fredrickson, Humberto S. Sanchez, Connie Chang, Diane Bimczok, James Wilking*
2:00 Paper 595e: Guest-Host Supramolecular Assembly of Injectable Hydrogel Nanofibers for 3D Cell Encapsulation and Pelvic Organ Prolapse Repair— ***Beverly Miller***, *Audrey Hansrisuk, Christopher B. Highley, Monique H. Vaughan, Steven Caliari*
2:18 Paper 595f: Continuous Chaotic Bioprinting of Pre-Vascularized Tissue Constructs — ***Edna Johana Bolívar-Monsalve***, *Carlos Fernando Ceballos-González, Brenda Guadalupe De la Cruz Rivas, Karen Ixchel Borrayo-Montaño, Anne-Sophie Mertgen, Juan Felipe Yee-de León, Carolina Chavez Madero, Ali Khademhosseini, Paul Weiss, Mario Moisés Álvarez, Grissel Trujillo de Santiago*
2:36 Paper 595g: Biofabrication of Muscle Fibers Enhanced with Plant Viral Nanoparticles Using Surface Chaotic Flows — ***Ada I. Frias-Sanchez***, *Diego Alonso Quevedo-Moreno, Mohamadmahdi Samandari, Jorge A. Tavares-Negrete, Víctor Hugo Sánchez Rodríguez, Ivonne González-Gamboa, Fernando Ponz, Mario Moisés Álvarez, Grissel Trujillo de Santiago*

(596) Biomaterials II

Thursday, Nov 11, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 105

Jorge Almodovar, Chair
Kelly Burke, Co-Chair
Kyung-Ho Roh, Co-Chair
Shreyas Rao, Co-Chair

Sponsored by: Biomaterials

12:30 Paper 596a: Isolation of Peptidoglycan from Hyperthemophillic Microorganisms for New Bioinspired Water-Responsive Materials — ***Malcolm Lane Gilchrist***, *Xi Chen*

12:48 Paper 596b: Rescue of Dendritic Cell Metabolism from Glycolysis Inhibition for Cancer Immunotherapy — ***Sahil Inamdar***, *Joslyn L. Mangal, Marion Curtis, Abhinav P. Acharya*
1:06 Paper 596c: Mechanical Characterization of Human Blood Via SPP Framework and Tevp Modeling — ***Matthew Armstrong***, *Arielle Zlotnick, Anthony Amaru, Jeffrey S. Horner, Kevin O'Donovan*
1:24 Paper 596d: Application and Characterization of Insect Repellent Containing Biopolymer Microcapsules As a Fabric Coating — ***James Ogilvie-Battersby***, *Rashmi Sharma, Ramaswamy Nagarajan, Ravi Mosurkal, Nese Orbey*
1:42 Paper 596e: Enhancing Prostate Cancer Immunity through the Rational Design of Vaccine Structure — ***Michelle Teplensky***, *Bin Zhang, Chad A. Mirkin*
2:00 Paper 596f: Engineering pH Sensitive Fusion Protein Vesicles — ***Dylan Dautel***
2:18: Break
2:36 Paper 596h: The Effect of Heparin/ Poly(L-Lysine) Layer-By-Layer Coating in Immunomodulatory Functions of Mesenchymal Stromal Cells Stimulated By IFN-γ — ***Mahsa Haseli***, *Jorge Almodovar*

(597) Catalysis in Liquid Media I

Thursday, Nov 11, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 203

Neeraj Rai, Chair
Nirala Singh, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

12:30 Paper 597a: Explaining the Activity Dependence on Particle Size for Phenol Hydrogenation on Pt and Rh By Identifying the Active Facet — ***James Akinola***, *Isaiah Barth, Jonathan Lee, Udishnu Sanyal, Oliver Gutiérrez-Tinoco, Bryan Goldsmith, Nirala Singh*
12:48 Paper 597b: Liquid Phase Effects on Adsorption Processes in Heterogeneous Catalysis — *Mehdi Zare,* ***Andreas Heyden***
1:06 Paper 597c: Spontaneous Electric Fields Play a Key Role in Thermochemical Catalysis at Metal-Liquid Interfaces — ***Thejas Wesley***, *Yuriy Roman, Yogesh Surendranath*
1:24 Paper 597d: Continuous Aqueous Flow Conversion of Dihydroxyacetone into Lactic Acid over Metal Phosphates. — ***Giada Innocenti***, *Eleni Papadopoulos, Giuseppe Fornasari, Fabrizio Cavani, Andrew Medford, Carsten Sievers*
1:42 Paper 597e: Understanding the Effects of Bromide Adsorption on the Direct Synthesis of H_2O_2 on Pd Nanoparticles — ***Pranjali Priyadarshini***, *Tomas Ricciurdulli, Jason Adams, Yang Sik Yun, David Flaherty*
2:00 Paper 597f: A Combined DFT and Classical Force-Field Approach for Modeling Kinetics of Acid-Catalyzed Reactions in Mixed Solvents. — ***Hoang Tran***, *Michael Janik, Scott T. Milner*
2:18 Paper 597g: Alcohol Solvent Effects in Glucose Isomerization in MOF Uio-66 — ***Roshan Ashokbhai Patel***, *Matheus Dorneles de Mello, Tyler Josephson, Michael Tsapatsis, Joern Siepmann, Matthew Neurock*
2:36 Paper 597h: Selective Electrochemical Reductive Amination of Benzaldehyde Using a Silver Catalyst — ***Zachary Schiffer***, *Minju Chung, Katherine Steinberg, Karthish Manthiram*

(598) Catalyst Design, Synthesis, and Characterization IV - Structure/Activity relationships studies II

Thursday, Nov 11, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 205

Canan Sener, Chair
Saurabh Bhandari, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

12:30: Break
12:50 Paper 598b: Morphology-Directed Restructuring of Core@Shell Nanoparticles: A Catalyst Design Strategy to Improve Material Utilization— ***Alexander Hill***, *Adarsh Bhat, Galen Fisher, Andrej Lenert, Johannes Schwank*
1:10 Paper 598c: Rational Design of PGM-Spinel Oxide Catalysts for Enhanced Methane Conversion — ***Debtanu Maiti***, *Kyle Karinshak, Karun Kumar Rao, Ru-Fen Liu, Michael Harold, Lars Grabow*
1:30 Paper 598d: Repurposing Organic Structure-Directing Agents for *a Priori*Control of Chabazite Zeolite Phase and Its Application to Methanol-to-Olefin Reaction — *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*
1:50: Break
2:10 Paper 598f: Intermediate Species, Active Sites, and Reaction Rate Constants in Heterogeneous Catalysis from Modulation Excitation Spectroscopy— ***Juan J. Bravo-Suárez***, *Hongda Zhu, Priya D. Srinivasan, Alejandra Torres-Velasco, Bhagyesha Patil*
2:30 Paper 598g: Single Atom Catalyst for Oxidation - Understanding the Fundamentals of Synthesis and Reactivity — ***Shyam Deo***, *Linxi Wang, Nicholas Pantelis II, Kayla Eudy, Zayne Weber, Ahana Mukhopadhyay, Robert Rioux, Michael Janik*

(599) Chemical and Catalytic Conversions and Processes for Renewable Feedstocks

Thursday, Nov 11, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 312

Aida Amini Rankouhi, Chair
LiLu Funkenbusch, Co-Chair

Sponsored by: Sustainable Biorefineries

12:30 Paper 599a: Synthesis of Bio-Sourced 4,4'-Dimethylbiphenyl — ***Mi Jen Kuo***, *Hong Je Cho, Yannick Kurz, Raul Lobo*
12:45 Paper 599b: Meso-Scale Studies of Simultaneous-Isomerization-Reactive-Extraction of Glucose to Fructose in a Flow Reactor — ***Ravikumar Gogar***, *Jeremy Schreur, Sridhar Viamajala, Patricia Relue, Sasidhar Varanasi*
1:00 Paper 599c: Hydrolysis of Bio-Oil Anhydrosugars Derived from Autothermal Pyrolysis of Cellulosic Biomass — ***Arpa Ghosh***, *Jake K. Lindstrom, Jessica Brown, Ryan G. Smith, Robert Brown*
1:15: Break
1:30 Paper 599e: Preparation of Pt/ZrO_2 Catalyst with Different Morphologies for the Selective Hydrogenation of Vegetable Oil — ***Minghao Zha***, *Hao Yan, Yibin Liu, Feng Xiang, Chaohe Yang*
1:45 Paper 599f: Catalytic Transfer Hydrogenolysis of Bio-Derived Polyols to High Value-Added Chemicals over Ru-Based Catalysts: Strain Effect and Structure Sensitivity — ***Wenxiang Zhang***, *Yanan Zhu, Dongpei Zhang, Yu Xiao, Yiyao Du, Jiefeng Liu, Jinyao Wang, Quanxing Zhang, Bin Yin, Guangyu Zhang, Mengyuan Liu, Chaohe Yang, Xin Jin*
2:00 Paper 599g: Aqueous Phase Reforming of Glycerol for Production of Hydrogen over Non-Noble Metal Nano-Catalysts — ***Liu Jiefeng***, *Yu Xiao, Jinyao Wang, Yushan Li, Guangyu Zhang, Mengyuan Liu, Dongpei Zhang, Yiyao Du, Wenxiang Zhang, Chaohe Yang, Xin Jin*

(600) CO_2 Capture By Adsorption II

Wednesday, Nov 10, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 309

F Handan Tezel, Chair
Masoud Jahandar Lashaki, Co-Chair

Sponsored by: Adsorption and Ion Exchange

3:30 Paper 600c: Low-Cost Nitrogen-Doped Activated Carbon Derived from Naturally Occurring Waste Leaves and Microalgae for CO_2 Capture — ***Salar Balou***, *Aashish Priye*
3:55 Paper 600a: Vapor Phase Infiltrated AlO_x/PIM-1 "Hybrid Scaffolds" As Solution-Processable Amine Supports for CO_2 Adsorption — *Fengyi Zhang, Emily McGuinness, Yao Ma,* ***Yi Ren***, *Johannes Leisen, Mark D. Losego, Ryan Lively*
4:20 Paper 600d: CO_2 Capture and Transport Behavior in MIL-101(Cr)-Amine Bearing Polymer Sorbents Under Unconventional Direct Air Capture Conditions— ***Guanhe Rim***, *Pranjali Priyadarshini, Cornelia Rosu, Fanhe Kong, Mingyu Song, Ryan Lively, Christopher W. Jones*
4:45 Paper 600g: A Comprehensive Overview of the Stability of Amine-Functionalized Carbon Dioxide Adsorbents — ***Masoud Jahandar Lashaki***, *Abdelhamid Sayari*
5:10 Paper 600e: Membrane Adsorbents Comprising Self-Assembled Inorganic Nanocages (SINCs) for Direct Air Capture — ***Thien Tran***, *Alisa Chakraborty, Timothy R. Cook, Haiqing Lin*
5:35: Break

(601) Effects of Confinement on Molecular Properties

Thursday, Nov 11, 12:30 PM
Marriott Copley Place, Salon H/I

Liqun Zhang, Chair
Liangliang Huang, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

12:30 Paper 601a: Molecular Dynamics Study of Asphalt-Water/Air Interface Systems — ***George Rucker***, *Liqun Zhang*
12:45 Paper 601b: Self-Diffusion of Mixtures of Hydrocarbon Gases and Liquids in Mesoporous Silicas with Different Pore Sizes By High Field Diffusion NMR— ***Blake Trusty***, *Samuel Berens, Pavel Kortunov, Hubert King, Sergey Vasenkov*
1:00: Break
1:15 Paper 601d: Novel Strategies for Fluid Confinement and Experimental Effects of Pressure-Driven Flow — ***Lani McKinnon***, *Bonan Wang, Hyeyoung Cho, Viktoriya Semeykina, Jules Magda, Milind Deo, Michael Bartyl, Ilya Zharov, Swomitra Mohanty*
1:30 Paper 601e: Interfacial Thermodynamics, Structure, and Dynamics of Imidazolium-Based Ionic Liquid-Oil Lubricants Under Confinement: Role of Surface Nano-Roughness and Temperature — ***Daria Lazarenko***, *Fardin Khabaz*
1:45 Paper 601f: The Behavior of Isopropanol in Nu-1000 MOF: Experiments and Molecular Dynamics Simulations — ***Madeleine Oliver***, *Liangliang Huang, Yao An, Yue Wu*

(602) Fundamentals of Catalysis and Surface Science III: Metal Oxides

Thursday, Nov 11, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 207

Tibor Szilvasi, Chair
Andrew R Teixeira, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

12:30 Paper 602a: Non-Faradaic Electrochemical Promotion of Brønsted Acid Catalysis — ***Alexander Khechfe***, *Mark Sullivan, Dimitrios Zagoraois, Alexandros Katsaounis, Constantinos Vayenas, Yuriy Roman*
12:48 Paper 602b: *Methyl Ketone Oxidative Scission over γ-Al_2O_3 Supported Vanadium Oxides: An Interpretation of Roles of Lattice Oxygen and Molecular Oxygen from Spectroscopic Insight* — ***Siwen Wang***, *Ran Zhu, Bowei Liu, Jesse Bond*
1:06 Paper 602c: Identifying Unique Interactions between Transition Metals and Perovskite Surface — ***Bader Alayyoub***, *Aleksandra Vojvodic*

1:24 Paper 602d: Carbonate Dimorphism, and the Interpretation of Rates of (Non)-Stoichiometric Oxygen-Driven Mars-Van Krevelen Redox Cycles — *Xiaohui Zhao, Qianyu Ning, Lars Grabow, Jeffrey Rimer, **Praveen Bollini***
1:42 Paper 602e: Effects of Framework Al Density in Chabazite Zeolites on Cu Ion Mobility and the Kinetics of NO_x Selective Catalytic Reduction with NH_3— ***Siddarth Krishna**, Casey B. Jones, Yujia Wang, Anshuman Goswami, David Dean, Jeffrey T. Miller, William Schneider, Rajamani Gounder*
2:00 Paper 602f: Probing the Atomic-Scale Effects of Surface Oxidation on Methanol Oxidation Reactivity By Cu Oxide Surfaces: A Combined Density Functional Theory and Surface Science Study — ***Alyssa Hensley**, Andrew Therrien, Renqin Zhang, Alex C. Schilling, Ryan Hannagan, E Charles Sykes, Jean-Sabin McEwen*
2:18 Paper 602g: Investigation of Pore Accessibility and Connections to Selectivity in Alkane Oxidation on M1 Phase Oxide — ***Adam Twombly**, Yilang Liu, Prashant Deshlahra*

(603) In Honor of the 2018 William H. Walker Award Winner II (Invited Talks)

Thursday, Nov 11, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 210

Justin Notestein, Chair
Rajamani Gounder, Co-Chair
Aditya Bhan, Co-Chair
David Flaherty, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

12:30 Paper 603a: Metal-Organic Frameworks Emerging As a Class of Well-Defined Solid Catalysts — *Dong Yang, **Bruce C. Gates***
12:50 Paper 603b: Acidity of Niobium Oxides from Catalytic Model Reactions Under Co-Presence of Water — ***Bo-Qing Xu***
1:10 Paper 603c: Challenges and Progress in Catalytic Upgrading of Liquefaction Intermediates from Biomass and Waste — ***Huamin Wang***
1:30 Paper 603d: Novel Catalysts for the Environmentally Friendly Synthesis of Methyl Methacrylate — ***Beata Kilos**, Chieh-Chao Yang, David G. Barton, Eric Weitz, Justin Notestein*
1:50 Paper 603e: Fundamental Insights into Reactions for Trace Contaminant Removal — ***Dante Simonetti**, Sara Azzam, Griffin A. Canning, Adam Hoffman, Alexey Boubnov, Philippe Sautet, Abhaya Datye, Simon Bare*
2:10 Paper 603f: Reactivity Descriptors for C-H Bond Activation and C-O Bond Formation in Hydrocarbons on Metal Oxide Catalysts — ***Prashant Deshlahra***
2:30 Paper 603g: Alkane Dehydrogenation Catalyzed By Brønsted Acidic and Reaction-Derived Carbonaceous Active Sites in Zeolites — *Philip M. Kester, Enrique Iglesia, **Rajamani Gounder***

(604) In Vitro and In Vivo Cancer Models

Thursday, Nov 11, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 109

Kaitlin Fogg, Co-Chair
Handan Acar, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

12:30: Break
12:48 Paper 604a: Engineering Ovarian Cancer Spheroids and Analyses of Drug Resistance and Migration — ***Gokhan Gunay**, Handan Acar*
1:06 Paper 629e: Circadian Regulation of Cytochromes P450 in 3D Hepatocarcinoma Spheroids — ***Vibha Narayanan**, André Lopes Rodrigues, Jonathan S. Dordick*
1:24 Paper 604c: Immunotherapy Combining IgG Opsonization and Macrophage Checkpoint Disruption Represses Growth of Cohesive Tumor Cell Clusters *in Vitro* and Solid Tumors in Mice — ***Lawrence J. Dooling**, Jason C. Andrechak, Brandon H. Hayes, Siddhant Kadu, Dennis E. Discher*
1:42 Paper 604e: Engineered Brain Microvascular Microenvironments Reveal a Role for Pericytes and Astrocytes in Shaping Vascular Architecture and Glioblastoma Behavior — ***Mai Ngo**, Brendan A. C. Harley*
2:00 Paper 604h: Peptide Frameworks for Screening the Effects of Amino Acids on Assembly — ***Handan Acar***
2:18 Paper 604g: Tissue-Inspired Synthetic Biomaterials (Invited Speaker)— ***Shelly Peyton***

(605) Interfacial Phenomena in Electrochemical and Electrokinetic Systems

Thursday, Nov 11, 12:30 PM
Sheraton Back Bay, Back Bay Ballroom A

Ariel Furst, Chair
Patricia Taboada-Serrano, Co-Chair

Sponsored by: Interfacial Phenomena

12:30 Paper 605a: Bridging the Gap between Electrokinetic Experiments and Molecular Dynamics Simulations — ***Max Döpke**, Remco Hartkamp*
12:45 Paper 605b: Investigating the Molecular Nature of Electrostatic Screening in the Double Layer — ***Aditya Limaye**, Karthish Manthiram, Adam P. Willard*
1:00 Paper 605c: Theory of Coupled Ion-Electron Transfer Kinetics— ***Dimitrios Fraggedakis**, Martin Z. Bazant*
1:15 Paper 605d: Quantitatively Deconvoluting the Influences of Electrolyte and Potential on Atomically Precise Catalysts at Electrified Interfaces — ***Joy Zeng**, Nathan Corbin, Kindle Williams, Karthish Manthiram*
1:30 Paper 605e: Isolation of Competing Patterns during Electrodeposition: Experiments Vs Theory — ***Sarathy Kannan Gopalakrishnan**, Akash Ganesh, Chun-Chieh Wang, Matthew Mango, Kirk J. Ziegler, Ranga Narayanan*
1:45 Paper 605f: Dynamic Processing of Electrodeposited Graded Density Alloys — ***Michael McBride***
2:00 Paper 605i: Electric Potential of Citrate Capped Gold Nanoparticles: Effects of Salt Concentration and Poly(Allylamine Hydrochloride) Wrapping— ***Xingfei Wei***
2:15 Paper 605h: Anion Effects on the Interfacial Structure and Bulk Physical Properties in Deep Eutectic Solvents — ***William Dean**, Burcu Gurkan*

(606) Lithium and Beyond: Fundamental Advances in High Performance Batteries II

Thursday, Nov 11, 12:30 PM
Sheraton Back Bay, Commonwealth

Joshua Gallaway, Chair
Shuya Wei, Co-Chair
Alexander Urban, Co-Chair
Nian Liu, Co-Chair

Sponsored by: Electrochemical Fundamentals

12:30 Paper 606a: Electrical Conductivities and Melting Points of Binary and Ternary Deep Eutectic Solvents Via Molecular Simulation — ***Gregory Opdahl**, Kenneth Benjamin*
12:45 Paper 606b: A Fully Integrated Experimental Platform for Benchmarking New Flow Battery Active Materials — ***Becca Segel**, Tejal Sawant, Thomas Henry, Carissa Yim, Zachary Parr, James R. McKone*
1:00 Paper 606c: Single-Ion Conducting Crosslinked Polymer Composite Gel Electrolytes — *Hunter Ford, **Emily Doyle**, David Webster, Peter Giannini,**Jennifer Schaefer***
1:20 Paper 606d: Operando Observation of Structural Evolution in Sulfur-Based All Solid-State Lithium Batteries — ***Alyssa Stavola**, Xiao Sun, Andrea Bruck, Daxian Cao, Hongli Zhu, Joshua Gallaway*
1:35 Paper 606e: Electrochemically Active ZnO Discharge Product Formed in Rechargeable Zn-Alkaline Batteries: Performance Effects and Mechanistic Insights — ***Brendan Hawkins**, Damon E. Turney, Gautam Yadav, Andrew M. Kiss, Timothy N. Lambert, Sanjoy Banerjee, Robert Messinger*
1:50 Paper 606f: Picoliter-Sized Zn-Air Batteries for Releasable Microscopic Sensors and Robots — ***Ge Zhang**, Volodymyr Koman, Matthias Kuehne, Jing Fan Yang, Michael S. Strano*
2:05 Paper 606g: Sodium-Ion Transport in $NaTi_2(PO_4)_3$ As an Electrode Material for Battery Applications: Insights from MD and DFT Simulations — *M. Ali Haider, **Deepak Seth**, Uzma Anjum, Manish Agarwal, Akshatha V, Aninda J. Bhattacharyya*
2:20 Paper 606h: Charge Storage Mechanisms of Quinone- & Flavin-Type Organic Electrodes for Rechargeable Aluminum Batteries Elucidated with Molecular-Level Specificity — ***Leo Gordon, MChem, MPhil**, Ankur L. Jadhav, Robert Messinger*

(608) Microporous and Mesoporous Materials II: Hydrocarbon Catalysis

Thursday, Nov 11, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 208

Michele Sarazen, Chair
David Hibbitts, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

12:30 Paper 608a: MOF-Supported Transition Metal Catalysts for 1-Butene Dimerization: A Mechanistic Study — ***Saumil Chheda**, Jian Zheng, Laura Löbbert, Navneet Khetrapal, Carlo A. Gaggioli, Julian Schmid, Oliver Gutiérrez-Tinoco, Ricardo Bermejo-Deval, Radha Kishan Motkuri, John L. Fulton, Mahalingam Balasubramanian, Matthew Neurock, Joern Siepmann, Laura Gagliardi, Johannes A. Lercher*
12:48 Paper 608b: Structural Change of Ferrierite during 1-Butene Isomerization at Extended Time on Stream — ***Karoline L. Hebisch**, Rick Watson, David Leyshon, Barbara Kimmich, Carsten Sievers*
1:06 Paper 608c: Role of Bronsted Acid Site Proximity in the Generation of Synergistic Sites for Alkane Cracking Conversion in MFI Zeolites — ***Tram Pham**, Vy Nguyen, Bin Wang, Steven Crossley*
1:24 Paper 608d: Fundamental Understanding of Structure, Location, and Stability of Zeolite-Supported Molybdenum Oxide Nanostructures for Methane Dehydroaromatization — ***Fateme Molajafari**, Joshua Howe*
1:42 Paper 608e: Propane Dehydrogenation and Cracking over Zinc-Exchanged H-MFI Zeolites Prepared By Solid-State Ion Exchange of Zinc Chloride — ***Danna Nozik**, Alexis Bell*
2:00 Paper 608f: Methanol-to-Olefins Catalysis in Erionite Molecular Sieves: Towards Enhancing the Ethylene Selectivity — ***Faisal Alshafei**, Youngkyu Park, Stacey Zones, Mark Davis*
2:18 Paper 608g: Accessibility and Reactivity of Protons in Sodalite Cages of Faujasite Zeolites — ***Xinyu Li**, Aditya Bhan, Michael Tsapatsis*
2:36 Paper 608h: Olefin Methylation Reactions over Iron Zeolites: Increasing Reaction Rates at Lower Temperatures and Shifting the Selectivity Towards Desired Products — ***Mark LaFollette**, Raul Lobo*

(609) Mixed-Matrix Materials for Gas Separation

Thursday, Nov 11, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 304

Michele Galizia, Co-Chair
Zachary Smith, Co-Chair

Sponsored by: Membrane-Based Separations

12:30 Paper 609a: Synthesis and Characterization of Multi-Dimensional Metal–Organic Frameworks for Efficient Gas Separations with Percolation Networks— ***Hyunhee Lee**, Won Seok Chi, Moonjoo Lee, Ke Zhang, Zachary Smith*

12:50 Paper 609c: Ultra-Permeable Mixed Matrix Membranes Based on PTMSP and Polymer Porous Networks with Enhanced Physical Aging Resistance — ***Jing Deng***, *Laura Matesanz Nino, Angel Lozano, Michele Galizia*
1:10 Paper 609d: Natural Gas Sweetening By Membranes — ***Yang Liu***, *John Yang, Sipei Li, Dana Wong*
1:30 Paper 609e: Peculiar Effect of Low Loading of Metal-Organic Polyhedra on CO_2/N_2 Separation Properties of Cross-Linked Polyethers — ***Taliehsadat Alebrahim***, *Liang Huang, Heshali Welgama, Vincent Pastore, Timothy R. Cook, Haiqing Lin*
1:50 Paper 609g: GPU-Empowered High-Throughput Screening of Metal-Organic Frameworks for Efficient Membrane Separation of C_2H_4/C_2H_6— ***Musen Zhou***, *Jianzhong Wu*

(610) Modeling, Estimation and Control of Industrial Processes

Thursday, Nov 11, 12:30 PM
Sheraton Back Bay, Back Bay Ballroom D

David Gay, Chair
Xunyuan Yin, Co-Chair

Sponsored by: Systems and Process Control

12:30 Paper 610a: Multistage Nonlinear Model Predictive Control of the Hydraulic Fracturing Process — ***Kuan-Han Lin***, *John P. Eason, Lorenz Biegler*
12:49 Paper 610b: Development of Koopman-Based Model Predictive Control with Multimodel Approach to Handle Local Dynamics of Chemical Processes in Presence of Feed Fluctuation — ***Sang Hwan Son***, *Hyun-Kyu Choi, Jiyoung Moon, Joseph Kwon*
1:08 Paper 610c: Distributed State Estimation from Delayed Measurements— ***Leila Samandari Masooleh***, *Jeffrey E. Arbogast, Ulku Oktem, Warren Seider, Masoud Soroush*
1:27 Paper 610d: Impact of Sensor Placement in Soil Water Estimation of Agro-Hydrological Systems: A Real-Case Study — ***Erfan Orouskhani***, *Soumya Sahoo, Bernard Agyeman, Song Bo, Xunyuan Yin, Jinfeng Liu*
1:46 Paper 610e: Mitigation of Fiber Degradation in a Pulp Digester Via Multiscale Modeling and Control of the Degree of Polymerization of Cellulose— ***Hyun-Kyu Choi***, *Sang Hwan Son, Joseph Kwon*
2:05 Paper 610f: Advanced Model Predictive Control for Reducing Equipment Damage in a Supercritical Pulverized Coal Fired Power Plant during Load-Following Operation — ***Elijah Hedrick***, *Katherine Reynolds, Sung Min Choi Hong, Debangsu Bhattacharyya, Stephen E. Zitney, Benjamin P. Omell*
2:24 Paper 610g: Reduced-Order Modeling of CFD and FEA Simulations for Predicting the Impacts of Control Actions and Cyberattacks on Materials — ***Kip Nieman***, *Matthew Wegener, Helen Durand*
2:43 Paper 610h: Optimal Sensor Network Design for Corrosion Monitoring of Multi-Scale Time-Varying Systems: Application to a Power Plant Boiler— ***Chandra Sekhar Somayajula***, *Debangsu Bhattacharyya, Xingbo Liu, Shanshan Hu*

(611) Novel Drug Carrier Formulations

Thursday, Nov 11, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 108

Abhinav P. Acharya, Co-Chair
Nisarg Shah, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

12:30: Break
12:48 Paper 611h: Biomaterials - an Immunometabolism Modulating Tool— ***Abhinav Acharya***
1:06 Paper 611b: Ultra-Deformable Liposomes for Enhanced Drug Delivery— ***Danielle Large***, *Debra Auguste*
1:24 Paper 611e: Multiscale Delivery and Bystander Effect of a Trop-2 Targeted Antibody Drug Conjugate with a Hydrolysable Linker — ***Anna Kopp***, *Shujun Dong, Scott Hofsess, Thomas Cardillo, Serengulam Govindan, Jennifer Donnell, Greg Thurber*
1:42 Paper 575f: Enhancing Macrophage Immunotherapy Via Supramolecular Nanoparticles for Dual Inhibition of CSF1R and MAPK Pathways — ***Anthony Brouillard***, *Anujan Ramesh, Sahana Kumar, Dipika Nandi, Ashish Kulkarni*
2:00 Paper 611h: Immune Responsive Biodegradable Materials — ***Nisarg Shah***
2:18 Paper 611g: Pathology Driven Approaches to Polymeric Drug Delivery to the Brain (Invited Speaker) — ***Jessica Larsen***

(612) Planning, Scheduling, Supply Chain and Logistics

Thursday, Nov 11, 12:30 PM
Sheraton Back Bay, Independence Ballroom West

Pedro Castro, Co-Chair
Maria Papathanasiou, Co-Chair

Sponsored by: Systems and Process Operations

12:30 Paper 612a: The Inherent Robustness of Closed-Loop (Online) Scheduling: Definitions, Algorithms, and Theoretical Guarantees — ***Robert McAllister***, *James Rawlings, Christos Maravelias*
12:49 Paper 612b: A Novel Two-Stage Scheduling Algorithm for Branched Pipeline Systems — *Yamin Yan,* ***Pedro Castro***, *Qi Liao, Yongtu Liang*
1:08 Paper 612c: Spatio-Temporal Economic Properties of Supply Chains— ***Philip Tominac***, *Victor M. Zavala*
1:27 Paper 612d: A Transactional Digital Twin for Optimizing Supply Chain Business Processes — ***Hector Perez***, *John Wassick, Ignacio Grossmann*
1:46 Paper 612e: A Platform for Online Inventory Optimization — ***Hector Perez***, *Christian D. Hubbs, Can Li, Ignacio Grossmann*
2:05 Paper 612f: Supply Chain Optimization for Modular Manufacturing with Production Feasibility Analysis Under Uncertainty — *Atharv Bhosekar,****Oluwadare Badejo***, *Marianthi Ierapetritou*
2:24 Paper 612g: Scheduling of Continuous Chemical Production Considering Transient Operations — *Yaqing Wu,* ***Christos Maravelias***
2:43 Paper 612h: Closed-Loop Integration of Scheduling and Offset-Free Model Predictive Control of Hydraulic Fracturing — ***Kaiyu Cao***, *Sang Hwan Son, Joseph Kwon*

(613) Polymer Thermodynamics and Self-Assembly

Thursday, Nov 11, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 104

Reza Foudazi, Chair
Andrew Peters, Co-Chair
Dong Meng, Co-Chair
Y. Elaine Zhu, Co-Chair
Kenneth Mineart, Co-Chair
Muzhou Wang, Co-Chair

Sponsored by: Polymers

12:30 Paper 613a: Block Copolymer Self-Assembly in the Presence of Liquid Crystals — ***Chinedum Osuji***
1:00 Paper 613b: Fouling Resistant Triblock Polymer Ultrafiltration Membranes with Tunable Pore Surface Properties — ***Wui Yarn Daphne Chan***, *Marc A. Hillmyer*
1:15 Paper 613d: High-Energy Density Shape Memory Polymers Using Strain-Induced Supramolecular Nanostructures — ***Christopher B. Cooper***, *Zhenan Bao*
1:30 Paper 613e: Anomalous Phase Formation in Spherical Block Copolymer Micelles in Low Intensity Magnetic Fields — *Karthika Suresh, Grace Kresge,****Michelle Calabrese***
1:45 Paper 613f: Solvent Controls Nanoparticle Size during Nanoprecipitation By Limiting Block Copolymer Assembly — ***Giovanni Bovone***, *Lucien Cousin, Fabian Steiner, Mark Tibbitt*
2:00 Paper 613g: What Insights Can Machine Learning Provide Towards Multiblock Copolymer Self Assembly? — ***Joshua Mysona***, *Juan J. de Pablo*
2:15 Paper 613h: Effects of Conformational Chirality on the Phase Behavior of Block Copolymers — *Natalie Buchanan, Julia Provenzano,* ***Poornima Padmanabhan***
2:30 Paper 613i: Molecular Simulation Investigations into the Root Causes of Bridge Defectivity in Block Copolymer Directed Self-Assembly — ***Jakin Delony***, *Sahar Zenoozi, Peter J. Ludovice, Clifford L. Henderson*
2:45 Paper 613c: Effect of the Shape and Relative Size of Building Blocks on the Properties of Hybrid Colloidal Gels — *Gelareh Rezvan, Mohsen Esmaeili, Monirosadat Sadati,* ***Nader Taheri-Qazvini***

(614) Process Monitoring & Fault Detection

Thursday, Nov 11, 12:30 PM
Sheraton Back Bay, Back Bay Ballroom C

Ravendra Singh, Chair
Mudassir Rashid, Co-Chair

Sponsored by: Information Management and Intelligent Systems

12:30 Paper 614a: OASIS-P: Operable Adaptive Sparse Identification of Systems for Fault Prognosis of Chemical Processing System — ***Bhavana Bhadriraju***, *Joseph Kwon, Faisal Khan*
12:45 Paper 614b: Health Monitoring of an Industrial Supercritical Pulverized Coal Boiler — ***Katherine Reynolds***, *Elijah Hedrick, Benjamin P. Omell, Stephen E. Zitney, Debangsu Bhattacharyya*
1:00 Paper 614c: Remaining Useful Life Prediction for a Reciprocating Compressor By a Data-Driven Model Based on an Operation Condition-Corrected Health Indicator — ***Jangwon Lee***, *Zhuoxiong Sun, Tai B. Tan, Jorge Mendez, Jesus Flores-Cerrillo, Jin Wang, Q. Peter He*
1:15 Paper 614d: Hidden Markov Model Based Fault Diagnoser Using Binary Alarm Signals with Estimated Confidence Levels — ***Joshiba Ariamuthu Venkidasalapathy***, ***Costas Kravaris***
1:30 Paper 614e: Machine Learning-Based Identification and Accommodation of Sensor Faults in Sampled-Data Process Systems — ***Amr Zedan***, ***Nael El-Farra***
1:45 Paper 614f: Fault Detection and Isolation in Uncertain Dynamic Systems Using Sensor Fusion and Inferential Sensing — ***Efi Safikou***, *William T. Hale, George Bollas*
2:00 Paper 614g: Data-Driven Subsystem Configuration and Distributed Process Monitoring — ***Xunyuan Yin***, *Yan Qin, Hongtian Chen, Jinfeng Liu, Biao Huang*
2:15 Paper 614h: An Integrated Fault Diagnostic Fault Prognostic Approach for the Health Condition Monitoring of Degrading Systems — ***Srikar Venkataraman Srinivas***, ***Iftekhar Karimi***

(616) Reaction Path Analysis I

Thursday, Nov 11, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 206

Hsi-Wu Wong, Chair
Andrew Adamczyk, Co-Chair
Toufiq Reza, Co-Chair
Prasanna Dasari, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

12:30: Break
12:45: Break
1:00 Paper 616b: General Prediction of Reaction Pathway Energetics on Alloy Surfaces Using a Latent-Variable Machine Learning Architecture — *Gbolade Kayode, Chukwudi F. Nwaokorie,* ***Matthew Montemore***
1:15: Break
1:30 Paper 616d: Mechanism for the Catalysis of Transesterification Using Homogeneous Tin — ***Charles J. McGill***, *Phillip Westmoreland*

1:45 Paper 616e: Transitory Sensitivities and Automated Analysis of Large Chemical Mechanisms — ***Matthew S. Johnson***, *William Green*
2:00 Paper 616f: Investigating the Formation of Aromatic Compounds during Methanol-to-Olefins in MFI Framework Zeolites — ***Hansel Montalvo-Castro***, *Mykela DeLuca, David Hibbitts*
2:15 Paper 616g: Effect of Surface Coverage on the Reduction of Carboxylic Acids on MoO_3 — ***Reda Bababrik***, *Laura Alejandra Gomez Gomez, Steven Crossley*

(617) Solid Form Selection: Cocrystals, Salts, Solvates, Polymorphs, and Beyond

Friday, Nov 19, 8:00 AM
Virtual, Separations Division (02)

Xiaobin Jiang, Chair
Gaurav Giri, Co-Chair

Sponsored by: Crystallization and Evaporation

8:00: Welcoming Remarks
8:03 Paper 617d: Mechanochemical Methods for Polymorphism and Salt/Co-Crystal Formation of Solid-State Pharmaceutical Applications — ***Qi Jiang***

(618) Structured Adsorbents: Beyond Pellets and Beads

Wednesday, Nov 10, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 311

Julien Cousin-Saint-Remi, Chair
Stefano Brandani, Co-Chair

Sponsored by: Adsorption and Ion Exchange

8:00 Paper 618a: Development of Expanded PTFE Structured Adsorbents with Parallel Channels — ***Sulaimon Adegunju***, *Ryan Sanders, Charles E. Holland, Armin Ebner, Guo Shiou Foo, Bob Grasso, Steve K. Stark, Joe W. Henderson, Jeff A. Knopf, James A. Ritter*
8:15 Paper 618c: Analysis of Direct Air Capture Process Conditions on Adsorptive Performance of 3D-Printed Aminosilica Monoliths — ***Kyle Newport***, *Shane Lawson, Ali Rownaghi, Fateme Rezaei*
8:30 Paper 618d: Development of a MOF-Textile Composite for Chemical Defense — *Meagan A. Bunge, Erick Pasciak, Jonglak Choi, Luke Haverhals, W. Matthew Reichert,* ***Thomas Glover***
8:45 Paper 618f: Demonstration of Engineered Structured Sorbents in Various Adsorption Applications — ***Kyle Hawley***, *Christian Junaedi, Codruta Zoican-Loebick, Subir Roychoudhury*
9:00 Paper 618g: Tvsa Cycle for Metabolic CO_2 Removal from Spacecraft Cabins Using a Structured Adsorbent: Bench Scale Parametric Study — ***Pravin B. C. A. Amalraj***, *Marjorie A. Nicholson, Armin Ebner, James A. Ritter*

(619) Surface Engineered and Responsive Membranes

Thursday, Nov 11, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 306

Dona Foster, Co-Chair
Ayse Asatekin, Co-Chair
Ranil Wickramasinghe, Co-Chair

Sponsored by: Membrane-Based Separations

12:30 Paper 619a: Enzyme-Functionalized PVDF Membrane Masks and Filters for Capture and Denaturation of Spike Glycoprotein for SARS-CoV-2 Deactivation — ***Rollie Mills***, *J. Todd Hastings, Thomas D. Dziubla, Yinan Wei, Dibakar Bhattacharyya*
12:55 Paper 619b: High-Performance Nanoparticle Capture Using Surface Functionalized Electrospun Cellulose Nanofilters — ***Shao-Hsiang Hung***, *Jared Bowden, Richard Peltier, Jessica Schiffman*
1:20 Paper 619c: High Performance Surface Nano-Structured Reverse Osmosis Membranes for Seawater and Brackish Water Desalination — ***Yian Chen***, *Yoram Cohen*
1:45 Paper 619d: Novel Electrospun Membranes for Membrane Distillation— ***Ranil Wickramasinghe***, *Yu-Hsuan Chiao*
2:10 Paper 619f: Biomimetic Scaffold for Smart Transportation — ***Katharina Cu***, *Anke Steier, Matthias Franzreb, Joerg Lahann*

(620) Sustainability and Consumer Products

Thursday, Nov 11, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 311

Jose Hernandez-Betancur, Chair
William Barrett, Co-Chair
Anh Tong, Co-Chair

Sponsored by: Sustainability Science and Engineering

12:30 Paper 620a: A Study of Thermal Management in Commercial Face Masks — ***Nabila Shamim***, *Utomwen Irabor, Ariful Bhuiyan*
12:45 Paper 620b: Synthetic biology platforms for the sustainable production of superior flavor and fragrance ingredients — ***Ernesto Simon***
1:00 Paper 620c: On the Quantitative Investigation of the Antimicrobial Efficacy of Grape Seed Extracts Against Food-Related Bacterial Pathogens. — ***Melina Kitsiou***, *Jorge Gutierrez-Merino, Katherine Costello, Simon Grewal,* ***Eirini Velliou***
1:15 Paper 620d: Systematic Screening of Materials for Consumer Products Using Semantically Enabled LCA — *Melina Psycha, Christos Mihalopoulos, Filopoimin Lykokanellos,* ***Antonios Kokosis***
1:30 Paper 722b: Innovating a Bendable Concrete Railroad Tie with Enhanced Fatigue Durability Via CO_2 Utilization — ***Weihsiu Hu***, *Duo Zhang, Victor C. Li, Brian R. Ellis*

(621) Sustainable Fuel from Renewable Resources

Thursday, Nov 11, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 309

Alvaro Orjuela, Chair
Lindsay Soh, Co-Chair
Juan-Gabriel Segovia-Hernandez, Co-Chair

Sponsored by: Sustainability

12:30: Break
12:50 Paper 621c: Aviation Fuel from Solar Energy: A Spain Supply Chain Network. — ***Andres Gonzalez Garay***, *Niall Mac Dowell, Nilay Shah*
1:10 Paper 621d: Production of Syngas Via Gasification Using Aspen Hysys Simulation — *Salih Rushdi,* ***Hayder Alhameedi***, *ASO Hassan, Hayder Al-Atabi, Zainab Al-Sharify, Joseph D. Smith*
1:30 Paper 621f: Feedstock Impact on Hydrothermal Liquification (HTL)— ***Michael R. Thorson***

(622) Synthetic Biology: Cell Free Systems, Biosensors, and Genetic Circuits

Thursday, Nov 11, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 110

Eric Young, Chair
Hyunmin Yi, Co-Chair

Sponsored by: Bioengineering

12:30 Paper 622a: A Low-Cost, Thermostable, Cell-Free Protein Synthesis Platform for on-Demand Production of Vaccines — ***Katherine Warfel***, *Michael Jewett*
12:48 Paper 622b: Leveraging Lipid-Protein Interactions to Engineer Spatial Organization in Cell-Free Systems — ***Justin Peruzzi***, *Timothy Vu, Jan Steinkuehler, Peilong Lu, David Baker, Neha Kamat*
1:06 Paper 622c: Development of a Naloxone Biosynthetic Pathway Using Cell Free Protein Synthesis and Deep Learning — *Sandra Vadhin, Zhiping Zhang,* ***Jeffrey D. Varner***
1:24 Paper 622d: Shifting Redox Reaction Equilibrium on Demand Using an Orthogonal Cofactor — ***Derek Aspacio***, *Edward King, William Black, Sean Perea, Han Li*
1:42 Paper 622e: High-Throughput Promoter Optimization for Improved Biobutanol *In Vivo* Biosensor — ***Nicholas Sandoval***, *Nancy Kim*
2:00 Paper 622f: Engineering Optogenetics in Red Yeast By Leveraging Transcriptomics and Modular Parts — *Joseph Collins, Emma Tobin, Anna Lipzen, Stephen Mondo, Igor Grigoriev,* ***Eric Young***
2:18 Paper 622g: Developing Portable, Shelf-Stable, on-Demand, and Cost-Effective Biosensors with Cell-Free Biosystems — ***Brad Bundy***

(623) Systems and Quantitative Biology: Microbial Traits, Regulation, and Interactions

Thursday, Nov 11, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 111

Junyoung Park, Chair
Daniel Woldring, Co-Chair

Sponsored by: Bioengineering

12:30 Paper 623a: A Semi-Synthetic Regulon in Saccharomyces Cerevisiae Identifies Factors Needed for Rapid Growth on Pentoses — ***Vikas Trivedi***, *Sean Sullivan, Debika Choudhury, Venkatesh Endalur Gopinarayan, Taylor Hart, Nikhil Nair*
12:48 Paper 160t: Leveraging Computational Stability and Ancestral Sequence Reconstruction As a Platform for the Site-Wise Diversification of the Haloalkane Dehalogenase Ligand Binding Pockets — ***Benedikt Dolgikh***, *James VanAntwerp, Jens Schmidt, Daniel Woldring*
1:06: Break
1:24 Paper 623d: Bacterial Persistence and Motility — ***Annie Lee***, *Pushkar Lele*
1:42 Paper 623e: *Escherichia coli* Nitric Oxide Detoxification Is Robust to Nitrogen Starvation — ***Xuanqing Wan***, *Mark Brynildsen*
2:00 Paper 623f: Syntrophic Consortia Enables Clostridium Ljungdahlii Growth Under Microaerobic Conditions — ***Anthony Stohr***, *Benjamin M. Woolston*
2:18 Paper 623g: Investigating and Targeting the Tactics Bacteria Use Against Phagosomal Stressors to Discover New Antibiotics — ***Mark Brynildsen***

(624) Transport Phenomena in Polymer Systems I

Thursday, Nov 11, 12:30 PM
John B. Hynes Veterans Memorial Convention Center, 103

Steven Lustig, Chair
Amanda Marciel, Co-Chair

Sponsored by: Polymers

12:30 Paper 624a: Understanding the Role of Crosslinks, Dynamic Bonds, and Specific Interactions on Mass and Ion Transport in Polymer Networks— ***Christopher Evans***
1:00 Paper 624b: Probing Ion Diffusion in Chemically Amplified Resists through Experiments and Atomistic Simulations — ***Christopher M. Bottoms***, *Tanguy Terlier, Gila E. Stein, Manolis Doxastakis*
1:15 Paper 624d: A Reaction-Diffusion Transport Model to Predict Precursor Uptake and Spatial Distribution in Vapor Phase Infiltration Processes — ***Yi Ren***, *Emily McGuinness, Chaofan Huang, Ryan Lively, Mark D. Losego*
1:30: Break
1:45 Paper 624f: Spatial Patterning of Dynamic Thermal Profiles Via Polymerization-Controlled Crystallization of Phase Change Materials — ***Thomas Schroeder***, *Joanna Aizenberg*
2:00 Paper 624g: Engineering Ion Transport in Polymer Membranes for Water Purification and Energy Applications — ***Geoffrey Geise***

2:15 Paper 624i: Sulfonated Poly(ionic liquid)s Block-Copolymers Membranes Based on Poly(styrene–isobutylene–styrene) for Chemical Protective Clothing— ***Karen Barrios Tarazona***, *David Suleiman*
2:30 Paper 624h: Degradation Pathways of Amine-Cured Epoxy Novolac and Bisphenol F Resins Under Conditions of High Pressures and High Temperatures— ***Narayanan Rajagopalan***, *Claus Erik Weinell, Kim Dam-Johansen, Søren Kiil*
2:45 Paper 649i: Sorption of Gaseous and Liquid Penetrants in Polyethylene Measured By Low Field NMR — ***Patrik Schneider***, *Tomáš Chaloupka, Martina Kukrálová, Juraj Kosek*

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

Friday, Nov 19, 12:30 PM
Virtual, Forest and Plant Bioproducts Division (17)

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

Sponsored by: Forest and Plant Bioproducts Division

12:30 Paper 625a: Natural Fiber Composites Using Seed Hulls from Grain Processing — ***Jagannadh Satyavolu***, *Kunal Kate*
12:50 Paper 625b: 3D Printed Biocomposites from Biocarbon and Polyamide 12 Via Selective Laser Sintering — ***Michael Snowdon***, *Benjamin Maldonado, Tao Wang, Amar K. Mohanty, Manjusri Misra*
1:10 Paper 625f: Evaluating durability after long-term thermal oxidation conditions of biocarbon filled biocomposites from polyphthalamide (PPA) and biobased polyamide (PA410) blend — ***Mateo Gonzalez De Gortari***, *Michael Snowdon, Amar K. Mohanty, Manjusri Misra*
1:30 Paper 625d: Biodegradable Plastic Blends and Organically Modified Nanoclay-Based Sustainable Nanocomposite Films for Packaging Applications— ***Akhilesh Pal***, *Feng WU, Manjusri Misra, Amar K. Mohanty*
1:50 Paper 625c: Biocarbon Production through Slow Pyrolysis of Chicken Feathers and Spent Coffee Ground Bio-Oil and Physicochemical Characterization of the Resulting Biocarbon — ***Ranjeet Mishra***, *Amar K. Mohanty, Manjusri Misra*

(626) Advances in mixed-integer optimization and optimization with logistics applications

Thursday, Nov 11, 3:30 PM
Sheraton Back Bay, Independence Ballroom West

Yash Puranik, Co-Chair
Philip Tominac, Co-Chair

Sponsored by: Systems and Process Operations

3:30 Paper 626a: A Network-Sampling Algorithm for the Solution of Large-Scale Supply Chain Models — ***Jiaze Ma***, *Philip Tominac, Victor M. Zavala*
3:49: Break
4:08 Paper 626c: Optimal Scheduling of Straight Multiproduct Pipelines with Automatic Batch Selection — ***Pedro Castro***
4:27 Paper 626d: Periodic Vehicle Routing with Trips Spanning Multiple Days— ***Aliakbar Izadkhah***, *Akang Wang, José Miguel Laínez-Aguirre, Jose M. Pinto, Chrysanthos Gounaris*
4:46 Paper 626e: Project Scheduling Algorithm Addressing Shared Due Dates— ***William Strahl***, *Chrysanthos Gounaris*
5:05 Paper 626f: Efficient Solution of Enterprise-Wide Optimization Problems Using Nested Stochastic Blockmodeling — ***Ilias Mitrai***, *Prodromos Daoutidis*
5:24 Paper 626g: A Distributed Optimization Framework for Cooperative Decision Making in Integrated Process Networks — ***Andrew Allman***, *Qi Zhang*
5:43 Paper 626h: Optimization Methods for the Integration of Spatially Explicit Landscape and Biofuel Supply Chain Network Design — ***Eric O'Neill***, *Christos Maravelias*

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

Thursday, Nov 11, 3:30 PM
Marriott Copley Place, Salon J/K

Yamil Colón, Chair
Obioma Uche, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

3:30 Paper 627a: Molecular Dynamics Simulations Uncover Mechanisms of Increased Stability in Binary Colloidal Suspensions of Microparticles and Nanoparticles — ***Vance Jaeger***, *Marzieh Moradi, Gerold A. Willing*
3:46 Paper 627b: Multidimensional Free Energy Landscapes for the Binding of Functionalized Nanoparticles to Lipid Bilayers — ***Jonathan Sheavly***, *Alex K. Chew, Reid Van Lehn*
4:02 Paper 627c: Molecular Dynamics Investigation of Crystal-Melt Interface Kinetics and Its Stability Limits during Horizontal Ribbon Growth of Silicon— ***Victor Fabiyi***, *Eunsu Paek*
4:18: Break
4:34 Paper 627e: Effect of Structural Variations of Sugar-Based Surfactants (alkyl polyglucosides) on Interfacial and Surface Tension — ***Harry Cardenas***, *Erich A. Muller, Sara Shahruddin, Jofry Othman, Siti Fatihah Salleh*
4:50 Paper 627f: How Radical Profiles in Particles Influence Emulsion Polymerisation? — ***Tomáš Chaloupka***, *Alexandr Zubov, Juraj Kosek*
5:06 Paper 627g: Facet-Selective Roles of Chloride and Polyvinylpyrrolidone (PVP) in Facilitating the Growth of Ag Nanowires and Nanocubes — ***Zihao Chen***, *Kristen Fichthorn*
5:22 Paper 627h: Computational Study of Coarse-Grained Ionic Liquids at Electrified Interfaces — ***Sergiy Markutsya***

(628) Biomaterial Scaffolds for Tissue Engineering II

Thursday, Nov 11, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 209

Gulden Camci-Unal, Chair
Mario Moisés Álvarez, Co-Chair
Samira Azarin, Co-Chair
Amol Janorkar, Co-Chair

Sponsored by: Biomaterials

3:30 Paper 628b: In Vitro Bone Model Capture Molecular Regulation of Bone Remodeling — ***Yongkuk Park***, *Jungwoo Lee*
3:48 Paper 628a: In Vitro Osteocyte Model Via Mechanoculturing Multi-Layered Bone Slices — ***Yongkuk Park***, *Jungwoo Lee*
4:06 Paper 628c: A 3D Hydrogel Culture System to Determine Impacts of Biomaterial Stiffness and Topographical Cues on Oligodendrocyte Progenitor Cell Viability, Growth and Differentiation — ***Rachel Mazur***, *Kyle Lampe*
4:24 Paper 628d: The Design and Fabrication of a Piezoelectric Biomaterial for Nerve Repair — ***Jacob Orkwis***, *Ann Wolf, Zach Mularczyk, Corinne Smith, Leyla Esfandiari, Greg Harris*
4:42 Paper 628e: Influence of Touch-Spun Fibers Diameter on Neurite Outgrowth and Schwann Cell Migration — ***McKay Cavanaugh***, *Darya Asheghali, Cecilia Motta, Elena Silantyeva, Matthew Becker, Rebecca Willits*
5:00 Paper 628f: Metabolite-Based Modulation of Dendritic Cells for Developing Effective Immunotherapy — ***Sahil Inamdar***, *Joslyn L. Mangal, Abhinav P. Acharya*
5:18 Paper 628g: Stiffness Induces Aging-like Phenotypic Changes in Microglia— ***Timothy Hackett***, *Srivatsan Kidambi*

(630) Catalysis in Liquid Media II

Thursday, Nov 11, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 203

Ali Hussain Motagamwala, Chair
Dezhou Guo, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

3:30 Paper 630a: Differences in Solvation Enthalpies and Entropies on Pt(111) Versus Pt/Al2O3 Particles and Their Influence on the Mechanism of Aqueous Phase Methanol Dehydrogenation — ***Ricardo Garcia***, *Bryan J. Hare, Carsten Sievers, Rachel Getman*
3:48 Paper 630b: The Nature of Acid Sites in MIL-100 Catalyzed Acetalization of Benzaldehyde with Methanol — ***Jacklyn Hall***, *Praveen Bollini*
4:06 Paper 630c: Solvent Molecules Form Surface Redox Mediators in Situ and Cocatalyze O_2 Reduction on Pd — ***Jason Adams***, *Ashwin Chemburkar, Pranjali Priyadarshini, Tomas Ricciurdulli, Yubing Lu, Vineet Maliekkal, Abinaya Sampath, Ayman M. Karim, Matthew Neurock, David Flaherty*
4:24: Break
4:42: Break
5:00 Paper 630f: Probing Surface-Adsorbate Interactions and Energetics through Active Particle Dynamics — ***Ben Greydanus***, *James Medlin, Daniel K. Schwartz*
5:18 Paper 630g: Substrate-Structure and Solvent Mediated Environment Around the Brønsted Acid Sites Governs the Dehydration Rate Enhancement of Alcohols inside Zeolite Confinements — ***Manish Shetty***, *Feng Chen, Huamin Wang, Oliver Gutiérrez-Tinoco, Donald M. Camaioni, Johannes A. Lercher*
5:36 Paper 630h: Understanding and Manipulating the Solvent Microenvironment for Selective, Catalytic Amination of Renewable Oxygenates— ***Dia Sahsah***, *Andreas Heyden*

(631) Catalyst Design, Synthesis, and Characterization V - Structure/Activity relationship studies III

Thursday, Nov 11, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 205

Matteo Cargnello, Chair
Nathaniel Eagan, Co-Chair
George Tsilomelekis, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

3:30 Paper 631a: Flame Aerosol Synthesis of Stable Ni/ZrO_2 Nanocatalyst for Dry Reforming of Methane — ***Shuo Liu***, *Mihir Shah, Junjie Chen, Satyarit Rao, Mohammad Moein Mohammadi, Eleni Kyriakidou, Mark Swihart*
3:50 Paper 631c: Gold Nanoparticles Directly Deposited inside Mesoporous SBA-15 Zeolites As an Active and Thermal Stable Catalyst — ***Zengran Sun***, *Steven Saunders*
4:10 Paper 631d: Effect of Metal Loading and Support Particle Size on the Catalytic Performance of Cs-Ru/CeO_2 in a Microwave Reactor for Ammonia Synthesis — ***Alazar Araia***, *Yuxin Wang, Jianli Hu*
4:30 Paper 631e: How Dry Should Dry Impregnation be? — ***Gregory Tate***, *Niklas Siebert, John Monnier, John R. Regalbuto*
4:50 Paper 631g: Using Ni@Pt Overlayer Catalysts for Dry Reforming of Ethane Reaction — ***Qian Yang***, *Josh Tepera, Teneil Schumacher, Jing Zhou, Joseph H. Holles*

(632) Chemical and Catalytic Conversions and Processes for Renewable Feedstocks II

Thursday, Nov 11, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 312

Aida Amini Rankouhi, Chair

LiLu Funkenbusch, Co-Chair

Sponsored by: Sustainable Biorefineries

3:30: Introductory Remarks
4:00 Paper 632c: Efficient Deoxygenation of Sludge Vegetable Oil over Bimetallic Doped Activated Carbon Catalyst for the Production of Green-Diesel-like Fuel — ***Alsultan Abdulkareem***, *Nurul Asikin Mijan, Siti Zulaika Razali, Robiah Yunus*
4:15 Paper 632d: Bio-Based Amines Production Via Selective Deoxygenation of N-Containing Biomass — ***Hongfei Lin***
4:30: Break
4:45 Paper 632f: The Role of Water in the Hydrodeoxygenation of 5-Hydroxymethylfurfural from Lignocellulosic Feedstocks — ***Zhaoxing Wang***, *Abhay Athaley, Marianthi Ierapetritou, Dionisios Vlachos*
5:00 Paper 632g: Nutrient Recovery and Fuel Precursor Production from Extracted Algae Residues Using Mild Oxidative Treatment — ***Tobias Hull***, *Jacob S. Kruger, Kameron Adams, Tao Dong, Nicholas J. Nagle, Philip Pienkos*

(633) Chemical Modifications and Processing of Biomaterials

Thursday, Nov 11, 3:30 PM
Marriott Copley Place, Suffolk

Zhaohui Tong, Chair

Sponsored by: Forest and Plant Bioproducts Division

3:30 Paper 633a: Conversion of Biowaste to Value-Added Biochemicals and Functional Biomaterials for High-Efficient Circular Economy — ***Zhaohui Tong***
3:45 Paper 633b: Microencapsulation of Flame Retardants Using Bio-Based Materials — ***Rashmi Sharma***, *James Ogilvie-Battersby, Jayant Kumar, Ravi Mosurkal, Nese Orbey, Ramaswamy Nagarajan*
4:00 Paper 633c: Impacts of High Shear-Rate Processing on Cellulose Nanofibrils — ***Bradley Sutliff***, *Aliya Kaplan, Samantha Stutz, Sam Oxley, Michael Bortner*
4:15 Paper 633d: Chitosan-Nanoparticle Enhanced Antibiotic and β-Lactamase Inhibitor to Treat Multi-Drug Resistant Pathogens — ***Arianna Partow***, *Zhaohui Tong*
4:30 Paper 633e: Tackling Water Pollution Via Sustainable Sorbents: Pb(II) Adsorption By Bio-Based Carbons Via First Principles Computational Models— ***Alyssa Hensley***, *Abisola Egbedina, Fanglin Che*
4:45 Paper 633f: Dewatering of Cellulose Nanofibers Using Ultrasound — ***Udita Ringania***, *Joseph Harrison, Robert Moon, M. Saad Bhamla*

(634) CO_2 Capture for Power Generation

Thursday, Nov 11, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 313

David Hopkinson, Chair
Zachary Smith, Co-Chair
Zi Tong, Co-Chair

Sponsored by: Sustainable Energy

3:30 Paper 634a: Supported Amine Adsorbents for CO_2 Capture Via Particle Molecular Layer Deposition — ***Hailey Loehde-Woolard***, *Annika Lai, William McNeary IV, Jessica Burger, Robert Pfeffer, Alan Weimer*
3:45 Paper 634b: Migration-Assisted Water Gradient Process for a Continuous CO_2 Capture — ***Rohan Sartape***, ***Aditya Prajapati***, *Meenesh Singh*
4:00 Paper 634c: Instantaneous Nucleation of Carbon Dioxide Hydrates Using Magnesium — ***Aritra Kar, MS***, *Palash Acharya, Awan Bhati, Ashish B. Mhadeshwar, Pradeep Venkataraman, Timothy Barckholtz, Hugo Celio, Filippo Mangolini, Vaibhav Bahadur*
4:15 Paper 634d: Mass Transfer Intensification Using 3D Printing Novel Dynamic Polarity Packing for Post Combustion Carbon Capture — *Min Xiao, Moushumi Sarma,* ***Jesse Thompson***, *Kunlei Liu*
4:30 Paper 634e: Systematic Chem-Informatics and Machine Learning Studies for Gas Permeability and Selectivity in Polymers — ***Wei Shi***, *Surya Tiwari, Samir Budhathoki, Janice A. Steckel, Ali Sekizkardes, Lingxiang Zhu, Shouliang Yi, Victor A. Kusuma, Kevin P. Resnik, David Hopkinson*
4:45 Paper 634g: Costs and CO_2 Sequestration Potential of Near-Term and Long-Term Implementation of Bio-Energy with Carbon Capture and Storage (BECCS) in the U.S. — ***Abishek Kasturi***, *Sotira Yiacoumi, Costas Tsouris, Joanna McFarlane, Ingrid Busch, Michael Hilliard, Matthew Langholtz*

(635) Data Science/Analytics for Process Applications

Thursday, Nov 11, 3:30 PM
Sheraton Back Bay, Back Bay Ballroom C

Salvador Garcia-Munoz, Chair
Kirti Yenkie, Co-Chair
Qi Zhang, Co-Chair

Sponsored by: Information Management and Intelligent Systems

3:30 Paper 635a: Managing Model and Data Alternatives within the Design of Ionic Liquid Enabled Separations of High Global Warming Potential Hydrofluorocarbon Refrigerants — ***Bridgette Befort***, *Alejandro Garciadiego, Gabriela Franco, Edward J. Maginn, Alexander Dowling*
3:45 Paper 635b: Data Analysis and Predictive Modeling for Wastewater Asset Management — ***Jake Stengel***, *Phuong Le, Nicolas Altieri, Emmanuel A Aboagye, Matt DeNafo, Dylan Bakley, Kirti Yenkie*
4:00 Paper 635c: Regularized Bayesian Fusion for Toxin Concentration Estimation in an Industrial Wastewater Treatment Plant — *Eugeniu Strelet,* ***Zhenyu Wang***, *You Peng, Ivan Castillo, Ricardo Rendall, Bea Braun, Mark Joswiak, Leo Chiang, Marco Reis*
4:15 Paper 635d: Model-Based Design of Experiments in Pyomo and Its Application to Adsorptive CO_2 Capture Systems — ***Jialu Wang***, *Alexander Dowling*
4:30 Paper 635e: Machine Learning-Based Soft Sensors for Vacuum Distillation Unit — ***Kamil Oster***, *Stefan Güttel, Lu Chen, Jonathan L. Shapiro, Megan Jobson*
4:45 Paper 635f: Statistical Machine Learning for the DOW Data Challenge Problem — ***S. Joe Qin***, *Siyi Guo, Zheyu Li, Leo Chiang, Ivan Castillo*
5:00 Paper 635g: Data-Driven Modeling and Optimization of an Industrial Scale Reverse Osmosis Desalination Plant — ***Marcello Di Martino***, *Styliani Avraamidou, Efstratios N. Pistikopoulos*
5:15 Paper 635h: Objective Assessment of Operator Training Using Correspondence Analysis of Physiological and Behavioral Measures— ***Mohammed Aatif Shahab***, ***Babji Srinivasan***, ***Rajagopalan Srinivasan***

(636) Delivery of Cancer Therapeutics

Thursday, Nov 11, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 108

Donald Belcher, Co-Chair
Michael Gower, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

3:30 Paper 636a: Leveraging Immortalized Brain Endothelial Cells to Enable High-Throughput, Preclinical Screening of Nanomaterials for Drug Delivery across the Blood Brain Barrier. — ***Nicholas Lamson***, *Andrew Pickering, Paula T. Hammond*
3:48 Paper 636b: A Cannabidiol-Loaded Mg–Gallate Metal-Organic Framework-Based Potential Therapeutic for Glioblastomas — ***Anu Sharma***, *Abhishek Kumar, Changning Li, Puja Panwar Hazari, Supriya D. Mahajan, Ravikumar Aalinkeel, Rakesh Kumar Sharma, Mark Swihart*
4:06 Paper 636c: Glucose Oxidase Delivery Using Polylysine-Grafted-Polyethylene Glycol Nanoparticles for Cancer Therapy — ***Saeed Manouchehri***, *Abanoub Hanna, Sarang Tartey, Ashish Ranjan, Joshua D. Ramsey*
4:24 Paper 636f: Alpha-Particle Nanotherapeutics Against Metastatic Triple Negative Breast Cancer — ***Aprameya Ganesh Prasad***, *Stavroula Sofou*
4:42 Paper 636e: ssDNA Nanotubes for Targeted Delivery of Doxorubicin to Triple Negative Breast Cancer Cells — ***Lucy Lin***, *Zachary Schneiderman, Efrosini Kokkoli*

(637) Development of Intermolecular Potential Models

Thursday, Nov 11, 3:30 PM
Marriott Copley Place, Salon H/I

Neeraj Rai, Chair
Nav Nidhi Rajput, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

3:30 Paper 637a: Revisiting the Trappe Force Field for Organophosphorus Compounds: Sarin, DMMP, and Dimp — ***Alina Emelianova***, *Elizaveta Basharova, Andrei Kolesnikov, Evaristo Villaseco Arribas, Ella Ivanova, Gennady Gor*
3:45 Paper 637b: Development of a Coarse Grained Discontinuous Molecular Dynamics Forcefield for Peptoids — ***Rakshit Jain***, *Carol Hall, Erik Santiso*
4:00 Paper 637c: Data-Driven Many-Body Models for Molecular Fluids— ***Francesco Paesani***
4:15 Paper 637d: Development of All-Atomistic Polarizable Force Fields for Molecular Simulations of Electronic Polarization Effects in Interfacial Phenomena — ***Rahul Prasanna Misra***, *Daniel Blankschtein*
4:30 Paper 637e: Benchmark of Topology Automated Force-Field Interactions (TAFFI) — ***Bumjoon Seo***, *Zih-Yu Lin, Qiyuan Zhao, Brett Savoie*
4:45 Paper 637f: Developing Phase-Transferable Machine Learning Force Fields of Molten Salts — ***Haimeng Wang***, *Ryan S. DeFever, Yong Zhang, Shobha Sharma, Matthew S Emerson, Claudio J Margulis, Edward J. Maginn*
5:00 Paper 637g: Interface Force Field for sp^3 Diamond Crystal Structures: Regression-Driven Development — ***Katarina Odak***, *Hendrik Heinz, Alan Weimer, Julie Nguyen*
5:15 Paper 637h: Integrated Strategy for Formulation of Realistic Potential Models for Simulation of Block Copolymers — ***Sahar Zenoozi***, *Nohemi Trevino-Garrido, Jakin B. Delony, Peter J. Ludovice, Clifford L. Henderson*
5:30 Paper 637i: Development of Coarse-Grained Forcefields for the Self-Assembly of Ceramide-Based Lipid Membranes — ***Christopher Iacovella***,***Parashara Shamaprasad***, *Chloe Frame, Annette Bunge, Clare McCabe*
5:45 Paper 637j: Development and Benchmarking of Small Molecule Force Fields in the Open Force Field Initiative — *John Chodera, Michael K. Gilson, David L. Mobley,* ***Michael Shirts***

(638) Fundamentals of Catalysis and Surface Science IV: Catalytic Mechanisms & Kinetics

Thursday, Nov 11, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 207

Alyssa Hensley, Chair
Alexander V. Mironenko, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

3:30 Paper 638a: Analysis of (side) Product Inhibition in the Measurement of Reaction Rates in Packed-Bed Flow Reactors: The Case of Ethane Partial Oxidation — ***Xiaohui Zhao***, *Jeffrey Rimer, Praveen Bollini*

3:48 Paper 638c: Elucidating the Role of Coadsorbed O/OH Species in the Selective Oxidation of Glycerol on Late Transition Metals — ***Geet Gupta***, *Luke Roling*
4:06 Paper 638d: 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*
4:24 Paper 638e: The Contribution of Acid and Redox Sites during the Catalytic Oxidation Scission of Ketones over Supported Vanadium Oxide: An in Situ FTIR Study. — ***Bowei Liu***, *Ran Zhu, Jesse Bond*
4:42 Paper 638f: An Analysis of Preferred Mechanisms of CO Oxidation in TiO_2-Supported Atomically Dispersed Catalysts Using the Energetic Span Model— ***Selin Bac***, *Nicholas Humphrey, Shaama Mallikarjun Sharada*
5:00 Paper 638g: N-Butane to 1,3-Butadiene Reaction over Pt Single Atoms in ZnO_x Nests in Dealuminated Zeolite Beta — ***Yanfei Zhang***, *Alexis T. Bell*
5:18 Paper 638h: Controlling the Adsorption-Induced Reaction Selectivity of Biphenyl-Based Molecules on Ag(111) — ***Dezhou Guo***, *Zhiwen Zeng, Jean-Sabin McEwen, Junfa Zhu*

(639) In Honor of the 2018 William H. Walker Award Winner III (Invited Talks)

Thursday, Nov 11, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 210

Aditya Bhan, Chair
David Flaherty, Co-Chair
Rajamani Gounder, Co-Chair
Justin Notestein, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

3:30 Paper 639a: Carbon Molecular Sieve Membranes: Tools for Engineering in Large Scale Gas Processing — ***William J. Koros***, *Zhongyun Liu, Wulin Qiu, Nicholas Leon*
3:50 Paper 639b: How to Write the Rate of a* + a* — *Neil Razdan,* ***Aditya Bhan***
4:10 Paper 639c: Charge of Reactive Hydrogen at Fluid-Transition Metal or Fluid-Transition Metal Sulfide Interfaces and Their Catalytic Roles in Hydrogenation and Hydrotreating Catalysis — *Junnan Shangguan, Haiting Cai, Alyssa Hensley, Haoyu Nie, Roberto Schimmenti, Matthew Gradiski, Robert Morris, Manos Mavrikakis, Jean-Sabin McEwen,* ***Ya-Huei (Cathy) Chin***
4:30 Paper 639d: In-Situ Promotion of Coupled Oxidation and Reduction Cycles over Metal Catalysts — ***Matthew Neurock***
4:50 Paper 639e: Mechanistic Insights into Acid Catalysis: The Myths and Challenges of Small Voids — ***Enrique Iglesia***

(641) Microporous and Mesoporous Materials III: Reaction Pathways and Effects Beyond the Binding Site

Thursday, Nov 11, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 208

Nicholas Brunelli, Chair
Jason S. Bates, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

3:30 Paper 641a: Ordered Hydrogen-Bonded Alcohol Networks Confined in Lewis Acid Zeolites Accelerate Transfer Hydrogenation Turnover Rates — ***Blake Johnson***, *John Di Iorio, Yuriy Roman*
3:48 Paper 641b: Computational Analysis of Monomer and Dimer Adsorption Trends in the MFI Framework — ***Pavlo Kostetskyy***, *Elsa Koninckx, Linda Broadbelt*
4:06 Paper 641c: Unraveling Complex Reaction Networks Combining DFT and Zeolite-Specific Kinetic Monte Carlo Simulations — ***Mykela DeLuca***, *Hansel Montalvo-Castro, David Hibbitts*
4:24 Paper 641d: Understanding the Adsorption Thermodynamics of Irreversibly Bound Adsorbates on Zeolite Surfaces — ***Ajibola Lawal***, *Omar Abdelrahman*
4:42 Paper 641e: Active Sites, Kinetics, and Second Sphere Coordination Effects for CO Oxidation on Mixed-Valence Oxo-Bridged Trimers — *Jacklyn Hall,* ***Praveen Bollini***
5:00 Paper 641g: Condition and Particle Size Effects on the Interconversion between Nanoparticles and Cations in Pd-Exchanged SSZ-13 Zeolites — ***Keka Mandal***, *Trevor Lardinois, Rajamani Gounder, Christopher Paolucci*
5:18 Paper 349h: Investigating the Consequences of Brønsted Acid Site Proximity on Propene Oligomerization in MFI Zeolites with DFT — ***Lauren Kilburn***, *Elizabeth Bickel, Rajamani Gounder, David Hibbitts*
5:36 Paper 641h: Effects of Intramolecular Forces & Solvent Mixtures on Epoxidations in Ti-Zeolites — ***David S. Potts***, *Daniel Bregante, Ohsung Kwon, David Flaherty*

(642) Polymers for Energy Storage and Conversion

Thursday, Nov 11, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 104

Shudipto K. Dishari, Chair
Joseph Stanzione III, Co-Chair
Iman Noshadi, Co-Chair

Sponsored by: Polymers

3:30 Paper 642a: The Importance of Polymer Electrolytes in Fuel Cell Electrodes in Meeting Performance and Durability Targets — ***Shawn Litster***
4:00 Paper 642b: An *in-Situ*-Polymerized Ionic Liquid Bridging Inter-Smectic Domain Gaps for Continuous Charge Transport Pathways As High-Performance Solid-State Electrolytes — ***Shuai Tan***, *Caihong Wang, Jie Luo, Yong Wu*
4:15 Paper 642c: The Role of Side-Chain Polarity on Conductivity and Thermal Stability in Molecularly Doped Conjugated Polymers — *Ban Dong, Christian Nowak, Jonathan Onorato, Tengzhou Ma, Christine Luscombe, Fernando Escobedo, Paul F. Nealey,* ***Shrayesh Patel***
4:30 Paper 642d: Tailoring Low Humidity and High Temperature Proton Conduction Using Cerium Oxide Based Nanocomposite Membranes — ***Varada Menon Palakkal***, *Gary K. Ong, Delia Milliron*
4:45 Paper 642e: Exposing the Interplay between Side Chain Sterics and Polarity in Conjugated Polymer-Based Redox Active Devices — ***Marlow Durbin***, *Anna Österholm, Alex Balzer, Lisa Savagian, John R. Reynolds, Natalie Stingelin*
5:00 Paper 642f: Selective Ion Conducting Polymers for Non-Aqueous Redox Flow Battery Applications — ***Geoffrey Geise***
5:15 Paper 642g: Mechanistic Elucidation of Conducting Binder for a Safer Potassium-Ion Battery Anode — ***Daniel Gribble***, *Vilas G. Pol, Bertan Ozdogru, Ömer Özgür Çapraz*
5:30 Paper 642h: An Artificial Layer Based on Polymer of Intrinsic Microporosity to Suppress Dendrite Growth on Li Metal Anode — ***Weixia Zhang***
5:45 Paper 642i: Synthetic Brochosomes As Ultra-Antireflective, Super-Hydrophobic Biomimetic Materials in Multifunctional Films for Electrochromic Applications — ***Progna Banerjee***, *Gabriel Burks, Marianne Alleyne, Mostafa Nassr, Sarah Bialik, Elizabeth Bello, Benny D. Freeman, Jeffrey E. Barrick, Charles M. Schroeder, Delia Milliron*

(643) Polymer Synthesis and Reaction Engineering

Thursday, Nov 11, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 105

Christian Pester, Chair
Jimmy Lawrence, Co-Chair

Sponsored by: Polymers

3:30 Paper 643a: Synthetic Approaches for the Generation of Diverse Sets of Polar Polyolefin Block Copolymers — ***Eva Harth***
4:00 Paper 643f: Kinetic Investigation on the Cationic Polymerization of Cyclic Poly(phthalaldehyde) — ***Anthony Engler***, *Paul A. Kohl*
4:20 Paper 643g: Solid-Supported Photoredox Polymerization Catalysis— ***Kirsten Bell***, *Christian Pester, Sarah Freeburne*
3:30 Paper 643i: Phase Inversion Prediction during the Bulk Synthesis of High-Impact Polystyrene: A Fluid-Dynamic Approach — ***Juan Maffi***, *Diana A. Estenoz*
5:00 Paper 643b: Enhancement on Alternating Copolymerization of Ethylene and Carbon Monoxide By Nickel-Based Catalyst — ***Bie Zhengwei***, *Bo-Geng Li, Zhen Yao*
5:20 Paper 643d: Engineering Polyolefin Thermoplastic Elastomers with Model-Guided Catalyst Feeding Policies Using a Tandem Polymerization — *Luo Liqiong,* ***Kan Liu***, *Jie Jiang, Qiulin Li, Pingwei Liu, Bo-Geng Li, Wen-Jun Wang*
5:40 Paper 643j: Elucidating the impact of side chain dispersity on the assembly of bottlebrush polymers at the air-water interface — *Nduka D. Ogbonna, Michael Dearman, Bhuvnesh Bharti, Andrew J. Peters, Andrew J. Peters,* ***Jimmy Lawrence***

(644) Predictive Control and Optimization

Thursday, Nov 11, 3:30 PM
Sheraton Back Bay, Back Bay Ballroom D

Helen Durand, Chair
Joel Paulson, Co-Chair

Sponsored by: Systems and Process Control

3:30 Paper 644a: Dual Adaptive Model Predictive Control with Disturbances— ***Zicheng Cai***, *B. Erik Ydstie*
3:49 Paper 644b: Development of Offset-Free MPC Framework for Hydraulic Fracturing Process Using Sindy — ***Parth Shah, Masters***, *Sang Hwan Son, Joseph Kwon*
4:08 Paper 644c: Deep Learning-Based Approximate Economic Model Predictive Control with Offset-Free Asymptotic Performance Guarantees Using a Modifier-Adaptation Scheme — ***Dinesh Krishnamoorthy***, *Ali Mesbah, Joel Paulson*
4:27 Paper 644d: Machine-Learning-Based Construction of Barrier Functions and Models for Safe Model Predictive Control — ***Scarlett (Siyao) Chen***, *Zhe Wu, Panagiotis D. Christofides*
4:46 Paper 644e: Efficient Coordination of Plantwide Distributed MPC: The Lyapunov Envelope Algorithm — ***Wentao Tang***, *Prodromos Daoutidis*
5:05 Paper 644f: Robust Explicit Model Predictive Control Via Robust Optimization — ***Iosif Pappas***, *Nikolaos A. Diangelakis, Richard Oberdieck, Efstratios N. Pistikopoulos*
5:24 Paper 644g: Integration of Scheduling and Optimal Control for Multi-Product Processes Using a Switched Dynamic System Formulation — *Oswaldo Andrés-Martínez,* ***Luis Ricardez-Sandoval***
5:43 Paper 644h: Offset-Free Koopman-Based Model Predictive Control of a Batch Pulp Digester — ***Sang Hwan Son***, *Hyun-Kyu Choi, Jiyoung Moon, Joseph Kwon*

(645) Reaction Path Analysis II

Thursday, Nov 11, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 206

Andrew Adamczyk, Chair
Hsi-Wu Wong, Co-Chair
Toufiq Reza, Co-Chair
Prasanna Dasari, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

3:30: Break
3:45: Break

4:00 Paper 645c: Applying Automated Reaction Prediction to Heterogeneous Catalysis Problems — ***Qiyuan Zhao***, *Yinan Xu, Jeffrey Greeley, Brett Savoie*
4:15 Paper 645d: Mechanistic Understanding of the Effect of Active Site Size in the Dehydrogenation of Ethane on Highly Dispersed Co/SiO_2 Catalyst— ***Sanjana Srinivas***, *Kewei Yu, Stavros Caratzoulas, Weiqing Zheng, Dionisios Vlachos*
4:30 Paper 645e: Data Driven Discovery of Reaction Pathways for Understanding Catalytic Cracking of Supercritical Dodecane in the Presence of ZSM-5 — ***Elizabeth Belden***, *Randy Paffenroth, Nikolaos Kazantzis, Michael T. Timko*
4:45: Break

(646) Sustainable Management and Uses of Post-Consumer Materials and Waste

Thursday, Nov 11, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 311

Damilola Daramola, Chair
Gerardo Ruiz-Mercado, Co-Chair
Jason Trembly, Co-Chair

Sponsored by: Sustainability Science and Engineering

3:30: Welcoming Remarks
3:45 Paper 646a: Waste Activated Sludge Valorization for Short-Chain Fatty Acids Production By Integrated Electro-Alkaline Treatment— ***Maasoomeh(Masi) Jafari***, *Gerardine G. Botte*
4:00 Paper 646b: pH Effects on Factors Influencing Nutrient Removal and Recovery from Synthetic Animal Waste Via Chemical and Electrochemical Techniques — ***Babatunde Ojoawo***, *Jason Trembly, Damilola Daramola*
4:15 Paper 646c: Systematic Evaluation of Emerging Wastewater Nutrient Removal and Recovery Technologies to Inform Practice and Advance Resource Efficiency — ***Anna Kogler***, *McKenna Farmer, Julia A. Simon, Sebastien Tilmans, George Wells, William Tarpeh*
4:30 Paper 646d: A Circular Economy Systems Engineering Framework for the Optimization of Food Supply Chains — ***Styliani Avraamidou***, *Stefanos Baratsas, Efstratios N. Pistikopoulos*
4:45 Paper 646e: Options for Reuse or Recycling of Wind Turbine Blades— ***Eberhard Lucke***
5:00 Paper 646f: Use of Responsible R2 (Reuse and Recycling) Practices for Sustaiable Ewaste Supply Chain — ***Ashit Dalal***

(647) Synthetic Biology: Tool and Method Development

Thursday, Nov 11, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 110

Nikhil Nair, Chair
Peng Xu, Co-Chair

Sponsored by: Bioengineering

3:30 Paper 647a: Developing a Fully Automated Workflow to Speed up the Design-Build-Test-Learn Cycle for Engineering of Microbial Cell Factories — ***Pu Xue***, *Huimin Zhao*
3:48 Paper 647b: Single-Particle Characterization of Engineered Extracellular Vesicles Using Halotag-Linked Fluorophores to Investigate Cargo Loading— ***Roxana Mitrut***, *Devin M. Stranford, Jonathan Chan, Muzhou Wang, Joshua N. Leonard*
4:06 Paper 647c: Engineering Dynamic Tuning of Gene Copy Number Via Plasmid Replication Control — ***Chenyi Li***, *Yusong Zou, Tian Jiang, Jianli Zhang, Yajun Yan*
4:24 Paper 647d: Dynamic Assembly of Cas6-Mediated RNA Scaffold for Colocalization of Enzymes in *Saccharomyces Cerevisiae*. — ***Anhuy Pham***, *Wilfred Chen, Nancy Da Silva*
4:42 Paper 647e: A Synthetic Biology Knowledge System Accelerates Design and Learning for Synthetic Biology Researchers — ***Kevin Keating***, *Jeanet Mante, Nicholas Rodriguez, Guarav Nakum, Jiawei Tang, Jacob Jett, Logan Terry, Eric Yu, Yikai Hao, Xiang Lu, Udayan Joshi, Brandon Sepulvado, J. Stephen Downie, Eric Young, Bridget McInnes, Mai Nguyen, Chris J. Myers*
5:00 Paper 647f: Developing a Highly Specific, Modular Platform for Conditional Protein Degradation — ***Hopen Yang***, *Wilfred Chen*
5:18 Paper 647g: Adding Valuable Functional Groups to Building Blocks Using New Synthetic Biology Tools — ***Aditya Kunjapur***

(648) Systems and Quantitative Biology: Modeling Biological Processes

Thursday, Nov 11, 8:00 AM
John B. Hynes Veterans Memorial Convention Center, 107

Rajib Saha, Chair
Christopher Kieslich, Co-Chair

Sponsored by: Bioengineering

8:00 Paper 648a: Systems medicine for revealing immunopathogenic mechanisms of age-dependent respiratory infection severity — ***Lauren Luciani***, *Jason E. Shoemaker*
8:18 Paper 648b: A Flight Simulator for Cancer Immunotherapy: Modeling CAR T-Cells in a Solid Tumor Context — ***Alexis Prybutok***, *Jessica S. Yu, Joshua N. Leonard, Neda Bagheri*
8:36 Paper 648c: Computational Modeling of the Relationship between Immune Cell Populations and the Bone Remodeling Cycle — ***Carley Cook***, *Brenda J. Smith*, ***Ashlee Ford Versypt***
8:54 Paper 648d: A Deep Learning Approach for Predicting Cell Motility States and Evaluating Cellular Heterogeneity — ***Debonil Maity***, *Hasini Jayatilaka, Nahuel Zamponi, Anjil Giri, Anshika Agrawal, Jeremy Walston, Denis Wirtz, Jude Phillip*
9:12 Paper 648e: Multicellular Spatial Model of RNA Virus Replication and Interferon Responses Reveals Factors Controlling Plaque Growth Dynamics — *Josua O. Aponte-Serrano*, ***Jordan Weaver***, *T.J. Sego, James Glazier, Jason E. Shoemaker*
9:30 Paper 648f: An Objective Method Screening Approach for Optimizing Cell Tracking and Identity Annotation in Dense Fluorescent Microscopic Images— ***Shivesh Chaudhary***, *Hang Lu*
9:48 Paper 648g: Using Modeling As Guide to Engineer Microbes for Industrial Applications — ***Gregory Stephanopoulos***

(649) Transport Phenomena in Polymer Systems II

Thursday, Nov 11, 3:30 PM
John B. Hynes Veterans Memorial Convention Center, 103

Steven Lustig, Chair
Amanda Marciel, Co-Chair

Sponsored by: Polymers

3:30 Paper 649b: Computational Study of Ion Transport in Polymer Electrolytes Near Glass Transition — ***Trung Nguyen***, *Monica Olvera De La Cruz*
3:45 Paper 649c: Evaluation of Surface Moisture Sorption and Diffusion in Materials — ***Hom Sharma***, *Brandon Foley, Pratanu Roy, Stephen Castonguay, Yunwei Sun, Elizabeth Glascoe*
4:00 Paper 649d: Multiscale Water Diffusion Measurements in Poly(ethylene glycol) and Glycerol Solutions — ***Joshua Moon***, *Thomas Webber, Dennis Robinson Brown, Peter Richardson, Thomas Casey, Songi Han, M. Scott Shell, Rachel Segalman*
4:15 Paper 649e: Solute Diffusion in Aliphatic Oil-Based Block Copolymer Gels— ***Kenneth Mineart***
4:30 Paper 649g: Vanadium Ion Dynamics of Ionomer-Nanoparticle Hybrid Membranes — ***Xueting Wang***, *Mayura Silva, Madhu S. Tyagi, Stephen Creager, Eric M. Davis*
4:45 Paper 649h: Influence of Charge Fraction on Transport of Penetrants through Polyelectrolyte Brushes — ***Shahryar Ramezani Bajgiran***, *Amanda Marciel*
5:00 Paper 649f: Predicting Volatile Emissions from Automotive Sealants and Empirical Correlations for the Key Mass Transfer Parameters for Phthalate Emissions from PVC Materials — ***Mary Gilliam***
5:15 Paper 694i: Nexar Block Copolymer Coated Composite Hollow Fiber Membrane for Liquid Desiccant Membrane Air Dehydration — ***Lakshmeesha Upadhyaya***, *Abaynesh Yihdego Gebreyohannes, Omar Abdelaziz, Suzana P. Nunes*
5:30 Paper 649a: Ion Transport in Polymer Electrolytes - Role of Ion Solvation and Dynamics — ***Shrayesh Patel***
Adsorption — *Christian Villa Santos*, ***Yamil Colón***
2:10 Paper 582c: Temperature Extrapolation of Henry Law Constants: Expanding the Thermodynamic Space of Adsorbent Screening — ***Daniel Siderius***, *Harold Hatch, Vincent K. Shen*
2:30 Paper 582e: Comparison of Fluorine Functionalization Strategies in MOFs for the Removal of Poly- and Perfluoroalkyl Substances from Water — *Turan Selman Erkal*, ***Ozgur Yazaydin***
2:50 Paper 582f: Towards Process-Materials Co-Optimization: Automatic Generation of Optimizable MOF Structure-Function Relationships — ***Xiangyu Yin***, *Lorenz Biegler, Chrysanthos Gounaris*