

November 5 - 10, 2023 Hyatt Regency Orlando • Orlando, FL

# LEADING THE WAY TO A SUSTAINABLE FUTURE

November 5 — November 10, 2023 Hyatt Regency Orlando Orlando, FL



**TECHNICAL SESSIONS** 2023

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

Sunday, Nov 5, 9:30 AM Hyatt Regency Orlando, Bayhill 22

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

**Sponsored by:** Professional Development Committee Liaison

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

Sunday, Nov 5, 1:00 PM Hyatt Regency Orlando, Regency Ballroom R/S

Roman Voronov, Chair Sundararajan Madihally, Co-Chair

**Sponsored by:** Meet the Candidates Poster Sessions

Poster 2b: Machine Learning Based Meta-Analysis of the Association between HLA-Peptide Binding Interactions and HLA-Linked Disease Susceptibility — Hyeju Song, Christopher Kieslich

Poster 2c: Sustainable Wastewater Treatment Technology: Application of Bio-Electrochemical Membrane Process — *Maryam Amouamouha* 

Poster 2d: Designing Colloidal Particles for Complex Self-Assembly Behavior — *Hillary Pan, Julia Dshemuchadse* 

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

Poster 2f: Tracking the Dynamics of Metal Nanomaterial to Improve Catalyst Design for Sustainable Fuel Production — *Johanna Schroeder*  Poster 29: Developing Nanoscale Tools to Advance Maternal, Fetal, and Neonatal Health — *Andrea Joseph* 

Poster 2h: A Facile Structural Engineering of Metal-Organic Frameworks for Enhanced Gas Separation Performance - Heseong An

Poster 2: Metabolic Engineering to Produce Gene Therapies and Therapeutic Biomolecules - Miguel Santoscoy

Poster 2j: Multi-Scale Disease Profiling Using Molecularly Programmable Tools — *Shih-Ting* (christine) Wang

Poster 2I: High Density Soft Electronic Fibers — *Muhammad Khatib* 

Poster 2m: Application of Quantum Materials in Dynamic Catalysis – *Richard Tran* 

Poster 2n: Advancing Biomass As Renewable Energy: Investigating Syngas Inhibition, Reaction Rate, and Reactor Simulation for Enhanced Hydrogen Production Via Steam Gasification — *Jieun Kim* 

Poster 20: Nano Biomanufacturing for Medicine and the Environment - Navid Bizmark

Poster 2p: 3D Printing across Length Scales and Material Classes for Energy, Environmental, and Health Applications – Max Saccone

**Poster 2q:** Development of Multi-Functional Materials for a Defossilized Carbon Economy

— Chae Jeong-Potter

Poster 2s: Precise Manufacturing of Advanced Materials Driven By Atomic Scale Characterization - Prashant Kumar Poster 2t: Protein- and Virus-Based Materials for Environmental and Agricultural Applications - Adam Caparco, Nicole F. Steinmetz

Poster 2u: Engineering Diagnostics for Mental Health Monitoring – *Marjon Zamani* 

Poster 2v: Hit the Lights: Developing Multiplex, Multichromatic Optogenetic Circuits for Cell Signaling and Tissue Engineering Applications – James Tang

Poster 2w: Development of Computational Tools for Peptoid Structure-Property Prediction - Rakshit Jain, Carol Hall, Jacqueline Hughes-Oliver, Erik Santiso

Poster 2x: Mesoscale Self-Organization of Biomolecular Condensates – *Sam Wilken* 

**Poster 2y:** Enhancing the Sustainability of Produced Water Treatment: Integrated EC-MF-Mdc System for Membrane Distillation with Crystallization

Chidambaram
Thamaraiselvan, Chhabilal Regmi,
Ranil Wickramasinghe

Poster 2z: Sustainable Polymeric Membranes for Molecular Separation- Greener Approach Towards Net Zero Emission - Lakshmeesha Upadhyaya

Poster 2aa: Architecting Functional Colloidal Materials *Via* Non-Equilibrium Interfacial Assembly — *Pavel Shapturenka* 

Poster 2ab: Belowground Carbon Farming: Engineering Genetic Circuits in Plant Roots and Rhizobacteria for Soil Carbon Sequestration — *Christopher Dundas*  Poster 2ac: Utilization of Renewable Energy Resources for New Energy Technologies: The Development of Cost-Effective and Stable Electro-Catalysts for Energy Conversion and Storage. – Syed Asad Abbas

Poster 2ad: Molecular Engineering of Reactive Electrochemical Interfaces – *Weilai Yu*, *Yi Cui, Zhenan Bao* 

Poster 2ae: Antibody-Conjugated Polymers and Nanoparticles for Targeted Chemo- and Immuno-Therapies — **Bin Liu** 

Poster 2af: Active Site Design That Traverses Catalytic Contexts - Joy Zeng

Poster 2ag: Advancing Materials Synthesis and Printing Technologies for Next-Generation Applications – *Shalinee Kavadiya* 

Poster 2ah: Monitoring Boron Concentration in Qatar Seawater and Its Impact on Desalination Processes – *Mosab Subeh* 

Poster 2ai: Engineering Biochemical Processes in Plant-Microbe Interactions for Sustainable Agriculture — *Kong Wong* 

Poster 2aj: Sustainable Chemistry with Machine Learning and Multi-Scale Simulations — *Aditya Dilip Lele* 

Poster 2ak: Cellular Control of Cu(l)-Catalyzed Alkyne-Azide Cycloaddition (CuAAC) Via Extracellular Electron Transfer in Complex Environments – *Gina Partipilo, Benjamin Keitz* 

Poster 2al: Transport-Directed Electrosynthesis for Decarbonization of Chemical Manufacturing – Justin Bui, Adam Z. Weber, Alexis T. Bell Poster 2am: Understanding Heterogenous Catalysis Via Multiscale Kinetic Simulation – Chuhong Lin

Poster 2an: Designing Membrane Systems for the Direct Separation of Multicomponent Organic Solvent Mixtures — *Hyeokjun Seo, Dong-Yeun Koh* 

Poster 2ao: Optimal Design of Soft Matter Via Simulation, Machine Learning and Large Language Models – *Jiale Shi* 

Poster 2ap: Biofuels, Biolubricants, and Biomaterials from Biomass and Energy-Efficient Ultrasonic Separation for the Sustainability and Decarbonization - Junli Liu

Poster 2aq: Accurate Computational Design of Programmable 3D Protein Crystals and Capsids — *Shunzhi Wang*, *Zhe Li, Isaac Lutz, Christoffer Norn, Una Nattermann, David Baker* 

Poster 2ar: Understanding and Controlling the Surface Physics and Chemistry of Complex Oxides - Abhinav S. Raman

Poster 2as: Carbon Capture and Utilization Using Non-Equilibrium Plasmas — *Hongtao Zhong* 

Poster 2at: Accelerated Materials Design and Discovery Using Self-Driving Laboratories. — *Kiran Vaddi* 

Poster 2au: Pressing Play on Self-Assembled Biomaterials — Shayna Hilburg

Poster 2av: Understanding Nanostructured Materials for High Catalytic Activities in Biosensors, Anti-Bacterial Activity, and Batteries — *Anuja Tripathi* 

Poster 2aw: Developing Computational Tools for *in silico* elucidation of Cancer Mechanisms, Microenvironment, and Drug Repositioning Candidates - Wheaton Schroeder

**Poster 2ax:** Multiscale Molecular Modeling in Porous Materials: A Comprehensive Approach Towards Accurate Predictions and Real Applications – *Filip Formalik*  **Poster 2ay:** Sustainable Catalysis for Carbon Waste Valorization: Integrating System and Molecular-Level Approaches – *Houqian Li* 

**Poster 2az:** Atomically Thin Membrane for Energy-Efficient Separation — *Shiqi Huang* 

Poster 2ba: Sustainable Chemical Manufacturing, Decarbonization, and Waste Management – Sean Najmi

Poster 2bb: Synthesis, Characterization, and Analysis of Non-Linear Polymers for Medicine - Zixian Cui

Poster 2bc: Physics-Based and Al-Driven Design of Functional Soft Materials — *Riccardo Alessandri* 

Poster 2bd: Designing Advanced Separation Processes for Critical Materials and Discovering Porous Membrane Materials for Sustainable Energy Applications – Xiaoyu Wang

Poster 2be: Multiscale Computational Design of Polymeric Materials for Sustainability and Healthcare – Heyi Liang

Poster 2bf: Developing Workflows to Understand and Design Complex Alloy Catalysts Using Density Functional Theory, Machine Learning, and Catalysis First-Principles – Gaurav Deshmukh

Poster 2bg: Computation and Theory-Guided Materials Discovery and Design for CO2 Capture, Utilization, and Storage – Bohak Yoon

Poster 2bh: Alkalide-Assisted Direct Electron Injection for the Noninvasive n-Type Doping of Graphene – Sanghwan Park, Chang Young Lee

Poster 2bi: Extremophile Stress Proteins for Engineering Novel Properties in Living Cells and Biomaterials – *Samuel Lim* 

Poster 2bk: Solar Thermochemical Fuel Production — *Remo Schäppi* 

Poster 2bl: Bridging the Gap between Structure & Function for Sustainable Carbonaceous Systems: An Analytical Multi-Scale Approach — *Heather LeClerc*  Poster 2bm: Advancements in Nanoengineering: Colloidal Soft Materials & Advanced Coatings for Energy and Bio-Applications - Shuhao Liu

Poster 2bo: A Data-Driven Approach to Materials Development for Emerging Separations Challenges - Matthew Rivera

Poster 2bp: Accelerating Transport Efficiency Via Active Motion: From Fundamentals to Practical Applications – *Haichao Wu* 

Poster 2bq: From Molecular Design to Macroscopic Properties: Interfacing Principles of Materials Chemistry, Molecular Self-Assembly, and Polymer Science for Sustainability — *Ty Christoff*-*Tempesta* 

Poster 2br: Modeling, Control and Optimization — Paulina Quintanilla

Poster 2bs: Exploiting Microbial Communities through Systems Biology and Synthetic Biology - Yiyi Liu

Poster 2bt: Penetration of Fluorescent Dye through Polymer Coatings – Krishnaroop Chaudhuri, Riddhiman Medhi, Zhenglin Zhang, Zhuoyun Cai, Christopher K. Ober, Jonathan Pham

Poster 2bu: Advanced Polymer-Derived Membranes for Pre-Combustion CO<sub>2</sub> Capture and Blue H<sub>2</sub> Production — *Leiqing Hu*, *Haiqing Lin* 

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

Poster 2bw: Barrier-Free Paper Analytical Devices for Multiplex Colorimetricdetection — *Ayushi Chauhan*, *Bhushan Toley* 

Poster 2bx: Automatic Reaction Mechanism Generation for Complex Systems Using Machine Learning and Computation – Matthew S. Johnson Poster 2by: Harvesting Cultivated Meat Grown in a Bioreactor with a Low Shear Centrifuge. Centrifuge Is Either Single Use or CIP/Sip. — David Richardson Sr.

Poster 2bz: Out-of-Equilibrium Generic Framework Predicts Concentration-Dependent Liquid Crystals – Jonathan Salmeron-Hernandez, Pablo Zubieta, Hans Christian Öttinger, Juan J. de Pablo

Poster 2ca: Enabling and Sensing Technologies for Healthcare, Environmental Monitoring, and Disease Control – *Mohammad Mofidfar* 

Poster 2cb: Targeted Degradation of Secreted and Cell Surface Proteins through the LRP-1 Pathway – *Elise Loppinet, Harrison A. Besser, Chaitan Khosla* 

Poster 2cc: Excipient-Based Strategy for Engineering Stable Ultraconcentrated Insulin Formulation – Yanxian Zhang

Poster 2cd: Transport of Soft Materials for Biomedical and Environmental Applications – *Jin Gyun Lee* 

Poster 2ce: Strain-Stiffening Modular Gels with Dynamic, Secondary Cross-Linking — **Sonu Kizhakkepura**, John Klier, Shelly Peyton

Poster 2cf: Solid Electrolyte Interphase: Where Polymer Composites Meet Electrochemistry - Huada Lian

Poster 2ch: Postdoc Candidate: Nanoscale Self-Assembly in Block Copolymer Blends — *Rahul Kumar*, *Henry Ashbaugh, Julie Albert* 

Poster 2ci: Biological Upcycling of Wastes for Sustainable Development — *Jinjin Diao*, *Tae Seok Moon* 

Poster 2cj: Selective Separation and Degradation of PFAS Using Redox-Based Polymers – *Paola Baldaguez Medina, Xiao Su* 

Poster 2ck: Guiding the Design of Energy Systems with Techno-Economic Assessment and Safety, Risk, and Reliability Analysis – Ahmad Al-Douri Poster 2cl: Conversion of END-of-Life Waste Streams to Low Carbon Fuels and Materials in a Circular Economy MODEL – *Emmanuel Galiwango, P.Eng., James Butler, Ma Weiguo, Samira Lotfi* 

Poster 2cm: Drug Delivery and Organismal Biophysics — *Pankaj Rohilla* 

Poster 2cn: Systems Engineering for Manufacturing of Advanced Biotherapeutics – *Francesco Destro* 

Poster 2co: Accelerated Energy Materials Discovery through Semiempirical Electronic Structure Methods — *Yeongsu Cho* 

Poster 2cq: From Causal Discovery to Multiscale Modeling in Biological Signaling Networks — *Robert Gregg* 

Poster 2cr: Innovating Light-Matter Coupling at the Nanoscale Interfaces – *Jingang Li* 

Poster 2cs: Build It up and Break It Down: Synthetic Biology and Biochemical Engineering for Sustainable Chemical Production and Bioremediation — *Jeremy David Adams* 

Poster 2ct: Molecular Engineering and Structural Design of Polymeric Materials for Energy-Water-Environment Nexus – *Youhong (Nancy) Guo* 

Poster 2cu: Understanding Gas Transport in Novel Membranes for Energy-Efficient Gas Separations: Polymers, Carbon Molecular Sieves, and Metal-Organic Frameworks – *Hyun Jung Yu* 

Poster 2cw: Chemical Systems Engineering for Water Solutions & Bioproducts Manufacturing - Remil Aguda

Poster 2cx: Real-Time Green CO2 Tracking with Artificial Intelligence in Biomass Co-Processing — Liang Cao, Bhushan Gopalunni, Yankai Cao

Poster 2cy: Miniaturized Systems. for Disease Management and Decentralized Diagnostics - Hanie Yousefi, Shana Kelley, Jonathan Rivnay, Edward Sargent Poster 2cz: Physics-Informed Material Discovery Tools for Energy and Space Applications - Maitreyee Sharma Priyadarshini

Poster 2da: Machine Learning Solutions to Complex Problems in Health, Environment, and Materials — Prateek Verma

Poster 2db: Adaptable Self-Driving Laboratories for Material Science and Chemistry — *Robert Epps* 

Poster 2dc: Miniaturized Systems for Disease Management and Decentralized Diagnostics - Hanie Yousefi

**Poster 2dd:** Microtubular Gas-Diffusion Electrodes for High-Efficiency Electrochemical CO<sub>2</sub> Reduction — *Hesamoddin Rabiee* 

Poster 2de: Developing a Sustainable Future through Research and Education in Synthetic Biology and Metabolic Engineering of Clostridia - Hyeongmin Seo

Poster 2df: Advancing Health and Sustainability through Multiscale Computational Modeling of Soft Materials – *Zhiqiang Shen* 

Poster 2dg: Utilization of Biomass-Based and Industrial Waste in 3D Printing Applications - Angi Ji

Poster 2dh: Investigation of the Impact of Sidechain Comonomer in the Ion Exchange Membrane (IEM) on the Electrochemical Cell Device Performance. — *Antara Mazumder* 

**Poster 2di:** Analysis and Design of Catalytic Reactions and Materials through Combined Experimental, Kinetic, and Computational Assessments — *Wenshuo Hu* 

Poster 2dj: Transport Phenomena and Materials Design in Electrochemical Renewable Energy Storage – *Zhifei Yan, Daniel G. Nocera* 

Poster 2dk: Unraveling Reaction Kinetics of Complex Systems for Sustainable Process Development - SriBala Gorugantu Poster 2dl: Computational and Experimental Investigation of the Distribution of Mo-Oxide Species in Mo/H-ZSM-5 — *Fateme Molajafari*, *Emanuele Joy, Rachita Rana, Simon Bare, Sheima Khatib, Joshua Howe* 

Poster 2dm: Decoding and Expanding Genome Functions for Living Technologies — *Anush Chiappino-Pepe*, *George M Church* 

Poster 2dn: Towards Next-Generation Non-Invasive Epidermal Biomedical Devices for Continuous Health Monitoring – Tamoghna Saha, Michael D. Dickey, Orlin D. Velev

Poster 2do: New Classes of Materials and Automated Experimental Design into Energy Storage Research – Juhyeon Ahn

Poster 2dp: Beyond Connectomic Imaging: Building an Integrative Platform to Investigate the Brain - Xiaotang Lu

Poster 2dq: Illuminating Neurochemical Signaling in the Brain with Near Infrared Nanosensors — *Natsumi Komatsu* 

Poster 2dr: Mulitscale Modeling of Interfacial Electrocatalytic Processes — *Nitish Govindarajan* 

Poster 2dt: The Ultra-Fast Dissolving Property of "Fenamates" Encapsulated Carbon Nanofibers (CNFs) for the Drug Delivery Application – Rupa Kasturi Palanisamy, Suresh Manivel, Torsten Stelzer, Carmel Breslin

**Poster 2du:** Bridging Biological Sequence and Molecular Function for Precision Diagnostics and Therapeutics – *Sevahn Vorperian* 

Poster 2dv: Bridging Physics-Informed and Data-Driven Materials Designs for Deep Decarbonization — *Jiayu Peng* 

Poster 2dw: New Data-Driven Modeling Paradigms in Systems Engineering Using Novel Neural Network Structures – Angan Mukherjee **Poster 2dx:** Rational Design of Sustainable Chemical Solutions with Reaction Networks and Data Science – *Evan Spotte-Smith* 

Poster 2dy: Peptide Guided Bio-Synthetic Composite Materials for Engineered Biointerfaces — *Tyler Jorgenson* 

Poster 2ea: Autonomous Bioelectronic Systems for Multiplex Functions – *Xu Zhang, Caroline M. Ajo-Franklin* 

Poster 2ed: Multiscale Engineering of Multiphasic Polymer Composites for Soft Electronics and Robotics – Samuel E. Root

Poster 2ec: Understanding and Engineering Sustainable Catalysis — *Selin Bac* 

Poster 2ee: Engineering Polymer Thin Films for Bio-Active and Energy Storage — *Pengyu Chen* 

Poster 2ef: High Density Soft Bioelectronic Fibers - Muhammad Khatib

Poster 2eg: Protein Engineering for Microbial Interface Study — *Zihang Su*, Julie Renner, Scott Banta

Poster 2eh: Re-Engineering Plasmonic Materials and Nucleic Acid across Different Length Scales for Advanced Catalysis and Biosensing – **Yifeng Shi**, Grigory *Tikhomirov* 

Poster 2ei: Design Principles and Mechanistic Understanding of Heterogeneous Catalysis Towards Sustainable Development – Md Delowar Hossain

Poster 2ej: Effect of CO2-Pretreatment on Reverse Water Gas Shift (rWGS) Using Ni-Doped CaTiO3/CaO — **Seongbin Jo**, Kandis Leslie Abdul-Aziz

Poster 2ek: Nano-Bio Interface Engineering with Precise Polymeric Nanostructures – *Beihang Yu* 

Poster 2el: Advanced Porous Materials for Molecular Discrimination of Light Hydrocarbons at Sub-Angstrom Precision — **Taehoon Hyun**, Dong-Yeun Koh Poster 2em: Overcoming Transport Barriers in Fluid-Solid Physical and Chemical Processes — Anthony Vallace

Poster 2en: Non-Equilibrium Dissipation As an Organizing Principle in Driven Soft Materials: From Polymers to Active Drops - Kailasham Ramalingam

Poster 2eo: Advancing Sustainable Chemistry through Experimental and Computational Approaches to Multi-Phase Chemical Reaction Processes – Ari Fischer

Poster 2ep: Charged Polymers and Granular Biomaterials for Biomedical Applications — Gabriel Rodriguez

Poster 2eq: Artificial Neural Network Model for Capturing the Effect of Local Atomic Environment on Surface Diffusion in Metals and Theirs Alloys — *Sandip Sawarkar* 

**Poster 2er:** Decarbonization of Fine Chemicals: Development of Alternative Pathways to Close the Carbon Cycle — *Juan Jimenez* 

Poster 2et: Development and Application of Surface-Active Nanoparticles – *Rong Ma* 

Poster 2eu: Tailoring Therapeutic Peptides to Enable Reversible Encapsulation into Different Drug Carriers — *Mark Bannon* 

Poster 2ew: Flow Chemistry-Enabled Sustainable Reaction Engineering – *Suyong Han* 

Poster 2ex: Engineering Polypeptides through Molecular Simulations, Machine Learning and Optimization Methods for Biological and Clean Energy Applications — *Yiming Wang* 

Poster 2ey: Builiding Nanomaterials for Energy Conversion and Energy Storage – *Dr. Aniket Sandip Mule* 

Poster 2ez: Next-Generation Bioelectronics Enabled By Single-Crystalline Inorganic Semiconductor Membranes - Jiho Shin, Jeehwan Kim, John A. Rogers

Poster 2fb: Engineering Hierarchical Materials for Structural Composites and Advanced Textiles – Lauren W. Taylor Poster 2fc: Hydrogel and Polymer Composite Materials for Water Treatment Technologies & Monitoring of Emerging Contaminants to Further the Understanding of the Environmental Exposome

— Angela Gutierrez

Poster 2fd: Synthesis and Computational Investigation of Novel Antioxidants Prepared By Oxidative Depolymerization of Lignin and Aldol Condensation of Aromatic Aldehydes – Daihong GAO, Xuebing Zhao

Poster 2fe: Selective Recovery of Pd<sup>2+</sup> from Spent e-Wastes *Via* Thermo-Responsive Poly(NIPAMco-14TCE-4)@PS Nanoparticles. — *Hiluf Tekle Fissaha* 

Poster 2ff: Laccase-Mediated Oxygen Reduction in Liquid Flow Fuel Cells for Efficient Oxidation of Biomass Derived Aldehydes with Co-Generation of Electricity - Nan Liu, Xuebing Zhao

Poster 2fg: Immunoengineering in Gut-Lung Axis — *Mohammad Aminul Islam* 

Poster 2fh: Advanced Material Systems That Harness Inhomogeneity and Multi-Scale Phenomena – *Tetsu Ouchi* 

Poster 2fi: The inside-out Lab: Engineering Microbial Communities from the inside-out - Jenna Ott

Poster 2fj: Thermochemical Processing of Biomass, Plastics and Waste Feedstocks - Harisankar S

Poster 2fk: High-Throughput Characterization of Transport Phenomena through Dynamic Membrane Systems – *Jonathan Ouimet* 

Poster 2fl: Jonathan Soucy: The Nerv Lab Will Excite Learning - Jonathan Soucy

Poster 2fm: Programming Nanoparticles: Inverse Design for Next-Generation Materials — *Timothy C. Moore* 

**Poster 2fn:** Developing Materials-Based Biointeractive Therapeutics and Technologies — *Sohyung Lee*  Poster 2fo: Dynamic Catalysts: Machine Learning Assisted Operando Characterization. — Prahlad Kumar Routh

Poster 2fp: Quick-Release Antifouling Hydrogels for Solar-Driven Water Purification - Xiaohui Xu, Rodney Priestley, Sujit Datta

**Poster 2fq:** Advancing PFAS Elimination through Catalytic Supercritical Water Reactors and Al-Enhanced Process Intensification — *Wenjia Wang* 

Poster 2fr: Microgel Surface Engineering to Enhance Cell Adhesion and Porosity of Injectable Granular Hydrogel Tissue Scaffolds – Jing Liu, Katie Li-Oakey, John Oakey

Poster 2fs: Towards Machine Learning Prediction of Kinetic Properties of Enzyme Variants - Veda Sheersh Boorla, Costas D. Maranas

Poster 2ft: Stimuli-Responsive Complex Fluids and Anisotropic Materials — *Tadej Emersic* 

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

Poster 2fw: Research and Teaching Interests of Andrew J. Fox - Modeling Multiphase Fluid Dynamics in the Inertial to Turbulent Regime — Andrew Fox

Poster 2fx: Design and Engineering of Molecules Using Molecular Simulations and Machine Learning — *Siva Dasetty* 

Poster 2fy: Engineering Tissue Physicochemical Properties for Multi-Omic Characterization — Seo Woo Choi, Kwanghun Chung

Poster 2fz: Leveraging Immunoengineering for Vaccine and Therapeutics Design – *Duo Xu* 

Poster 2ga: Active Matter and Liquid Crystals Under External Fields: Basic Science and Applications — *Antonio Tavera Vazquez*  Poster 2gb: Inverse Design of Complex Flow Systems Using Theory and Differentiable Direct Numerical Simulations – Mohammed Alhashim

Poster 2gc: Elasticity Induced Dynamics of Complex Fluids and Filaments – Manish Kumar

Poster 2gd: Atomic and Molecular Design of Materials for Sustainable Energy Storage Solutions – *Julia Yang* 

Poster 2ge: Multi-Fidelity Computer-Aided Molecular Design - Kevin P. Greenman

Poster 2gf: Probabilistic Prediction Model-Based High-Throughput Screening for Discovering Feasible and Effective Catalysts for Dry Reforming of Methane — *Hyundo Park, Jiwon Roh, Hyungtae Cho, Insoo Ro, Junghwan Kim* 

Poster 2gg: Heterogenization of Metallocene Catalysts over Surfactant Modified Layered Double Hydroxide Sheets for Efficient Olefine Copolymerization. – Hassam Mazhar, Mamdouh A. Al-Harthi

Poster 2gh: Exploring the Frontiers of Molecular Diffusion through Machine Learning-Based Forcefields and Electron Density Predictors — *Siddarth Achar, Karl Johnson* 

Poster 2gi: The Signal in the Noise: Fluctuations in Interfacial Chemistry, Quantum Molecular Machines and Photosynthesis — Amro Dodin

Poster 2gj: Simulation-Aided Energy and Economic Evaluation for Amine-Based CO<sub>2</sub> Capture Matching Existing Power and Industrial Processes – *Koki Yagihara*, *Kazuki Fukushima*, *Jialing Ni, Hajime Ohno, Yasuhiro Fukushima* 

Poster 2gk: Exploring the Potential Applications of Advanced Porous Nanomaterials for Real World Challenges: Molecular Simulations and Experiments - Mahdi Niknam

Poster 2gl: Bio Soft Materials for Advance Applications — *Diego Gomez-Maldonado*  Poster 2gm: Spatial and Temporal Control of Immunobiologics for Disease Treatment — *Parisa Yousefpour* 

Poster 2gn: Improving Biological Molecule Delivery through Understanding the Endomembrane System — *Ryan Splichal* 

Poster 2go: Rational Sustainable Polymer Materials Design Using Multiscale Simulation and Theory – Pierre Kawak, David S. Simmons, Douglas Tree

Poster 2gp: Driving Electron and Photon Induced Chemistries to Enable a Sustainable Economy - Samji Samira

Poster 2gq: Machine Learning-Assisted Multiscale Modeling for Materials Design — *Fangxi Wang* 

Poster 2gr: Cracking the Code: Engineering Extracellular RNA and Nanoparticle Trafficking to Control Host-Microbe Interactions – Angela Chen

Poster 2gs: Unleashing the Therapeutic Potential of Cells: Cellular Reprogramming and Tissue Engineering for Enhanced Function and Healing – *Pihu Mehrotra* 

Poster 2gt: Enabling Microscale Processing for Structured Healthcare Materials – Zehao Pan

Poster 2gu: Revolutionizing Tissue Repair with Advanced Functional Adhesives – *Aishwarya Menon* 

Poster 2gv: Engineering Complex Fluid-Fluid and Fluid-Solid Interfaces for Drug Delivery - Vineeth 'Vinny' Chandran Suja

Poster 2gw: Catalyst Design for Water Treatment Using *Ab Initio* Simulation — *Yu Chen, Thomas Senftle* 

Poster 2gx: New Dimensions in the Human Command of Matter Toward Sustainability — *Saman Moniri* 

Poster 2gy: Spectroscopic and Computational Study of Catalytic Nickel Nitride Structures for Plasma-Assisted Ammonia Synthesis – *Yiteng Zheng*  Poster 2gz: Computational Studies of the Structure and Dynamics of Biomolecules at Interfaces – *Faramarz Joodaki* 

Poster 2ha: Spectroscopic Imaging and Computational Chemistry at the Intersection of Biology and Material Science – Matthew Confer

Poster 2hb: Investigation of Breast Cancer Recurrence Mechanisms Following Radiotherapy of Mammary Gland Adipose Tissue: Evaluating Cellular Metabolism & 3D in Vitro Models — *Kevin Corn, Marjan Rafat* 

Poster 2hc: DFT and Classical MD: A Computational Toolkit to Study Electrocatalysis and the Electrode-Electrolyte Interface – Andrew Wong, Michael Janik

Poster 2hd: Upcycling of Plastics and Bio-Polymers: Design of Catalysts and Reactions – Jaeheon Kim

Poster 2he: Faculty and Post-Doc Candidate: Dr. Yaprak Ozbakir – Yaprak Ozbakir

Poster 2hf: Cellulose Based Anti-Fouling Coatings for Application in Medical Devices. — *Eric Walker* 

Poster 2hg: Model-Based Pharmaceutical Process Design - Ayse Eren

Poster 2hh: Big Data Analytics for Disease Systems Biology and Bioprocess Engineering - Saratram Gopalakrishnan

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Poster 2hi: Sustainable Chemical Manufacturing — *Arthur Shih* 

Poster 2hj: Bioinspired Soft Separation Materials and 2D Polymers – Yu-Ming Tu

Poster 2hk: Multi-Scale Processing of Architecturally Complex Polymer Materials - Michael Burroughs

Poster 2hl: Radiation Therapy Enhances Breast Cancer Cell Proliferation and Invasion in Extracellular Matrix Hydrogels – *Tian Zhu, Kevin Corn, Marjan Rafat* 

Poster 2hm: Non-Invasive Sensing and Actuation inside Biological Systems with Functional Soft Materials – *Yuxing Yao*  Poster 2hn: Translational Research for Auditory and Sensory Systems. — *Parveen Bazard* 

Poster 2ho: Scalable Ionic Polymer Thin Films for Iontronic Device Applications – *Kwang-Won Park* 

Poster 2hp: A Computationally Assisted Approach for Designing Wearable Biosensors Toward Non-Invasive Personalized Molecular Analysis – **Daniel Mukasa**, *Minqiang Wang, Jihong Min, Yiran Yang, Samuel Solomon, Hong Han, Cui Ye, Wei Gao* 

Poster 2hq: Rational Design of Polymers for Sustainable Water, Energy, and Environmental Separations – *Rahul Sujanani* 

Poster 2hr: Beyond Adsorbates: Tracking Dynamic Catalyst Reshaping to Uncover Hidden Structure-Function Relationships - Griffin A. Canning

Poster 2hs: Fabrication of Polymeric Systems for Biomaterials — *Keturah Bethel, Eric M. Davis* 

Poster 2ht: Rigorous Statistical Mechanics and Rare Events Tools to Model Catalyst Site Ensembles - Salman A. Khan

Poster 2hu: Carbon Capture and Aerosol Technology for Carbon Dioxide Utilization — Onochie Okonkwo

Poster 2hv: Computational Living Matter through the Lens of Biomolecular Condensates, Active Systems, and Data-Driven Learning — *Hongbo Zhao* 

Poster 2hw: Computational Modeling of Cellular Metabolism across Spatiotemporal Scales for Health and Biotechnology Applications. — *Tracy Kuper* 

Poster 2hx: Combined Synthetic and Kinetic Approaches for Understanding Catalytic Processes - Gregory Tate

Poster 2hy: NON-Oxidative Catalytic Cnversion of Methane into Benzene over Hierarchical Mo/HZSM-5 Catalyst – Deepti Mishra, Kamal Pant, Muxina Konarova Poster 2hz: Materials for a Sustainable Future: Understanding Electronic Structure & Engineering Electron Transfer to Design Materials for Sustainability - Subhajyoti Chaudhuri

Poster 2ia: Electrochemical Systems with Flowable Suspension Electrolytes for Sustainable Future – Madhu Venkata Rama Krishna Majji

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

Poster 2ic: Adhesion of Wet, Compliant and Rough Soft Materials – *Preetika Karnal* 

Poster 2id: Applications of Genome-Scale Modeling on Quantifying Metabolism and Strain Design — *Patrick Suthers* 

Poster 2ie: Electronic Waste Derived Three-Dimensional Carbon Aerogel for the Adsorption of Phenol from Wastewater — *Marut Jain* 

Poster 2if: Chemical Conjugation Strategies for Functional Intracellular Delivery of Protein Therapeutics – *Azmain Alamgir* 

Poster 2ig: Efficient, Scalable, and Sustainable Manufacturing of Polymer Composites and Applications in Fire Safety - Yufeng Quan, Qingsheng Wang

Poster 2ih: Harnessing Water Entropy and Electric Field to Design Aqueous Polymer Systems for Sustainability and Bioengineering — *Shensheng Chen* 

Poster 2ii: Materials for CO<sub>2</sub> Capture, Conversion and Storage — Nabankur Dasgupta, Tuan Ho, Adri C.T van Duin

Poster 2ij: Innovating Pharmaceutical Technology through Prototyping, Process Analytics and Modeling – *Ajinkya Pandit* 

Poster 2ik: Single-Step Aerosol Method for Scalable and Sustainable Valorization of Lignin - Sujit Modi, Pratim Biswas Poster 2il: Deep Learning-Enabled Design of Protein-Nucleic Acid Assemblies for Gene Regulation and Gene Therapy – *Cameron Glasscock* 

Poster 2im: Biomaterials of Tomorrow: Feedstock's Variability a Materials Challenge for Renewable Resources Engineering. — *Diana Ramirez Gutierrez* 

Poster 2in: Hydrogen Transfer-Mediated Chemical Transformation and the Coupled Physical Effects – Gang Wan

Poster 2io: Ultra-Flexible Endovascular Probes for Brain Recording through Micron-Scale Vasculature – *Angi Zhang* 

Poster 2ip: Engineering Biomaterials for Women's Health — Aida López Ruiz, Catherine Fromen, April Kloxin, Kathleen McEnnis

Poster 2iq: Integrated Functional Polymer Engineering Pipeline for Next-Generation Biotechnologies – Juhyuk Park, Kwanghun Chung

Poster 2is: Effect of the Concentration of Brönsted and Lewis Acidic Sites on the Main Reaction Pathways during the Conversion of Fructose over Sn-KIT-6-PrSO<sub>3</sub>h Bifunctional Catalyst

 Edgar Tututi, Horacio
González, Gutiérrez-Alejandre Aída, Jose L. Rico

Poster 2it: Immunoengineering Strategies for Neurological Diseases – *Rick Liao, Elizabeth Nance, Samir Mitragotri* 

Poster 2iu: Theoretical and Computational Approaches for Upscaling Nanoengineered Materials to Design High Strength Polymeric Structural Materials – Nitant Gupta

Poster 2iv: Computational Design of Materials for Energy Conversion and Storage – *Alexandra Zagalskaya* 

Poster 2iw: Energy System Decarbonization: Leveraging Optimization-Based Techniques for a Sustainable Future – *Kaiyu Cao* 

Poster 2ix: A Microfluidic Chip Structure with Ultra-High Liquid-Liquid Mass Transfer Performance – Jing Song Poster 2iy: Liquid Flow Fuel Cell with Modified Anode for Efficient Oxidation of 5-Hydroxymethylfurfural to Produce 2, 5-Furandicarboxylic Acid with Co-Generation of Electricity — Ye Qiang, Xuebing Zhao

Poster 2iz: Catalytic Microwave-Assisted Pyrolysis of Waste Plastics for Circular Economy Development — *Roger Ruan Sr.*, *Leilei Dai Sr.* 

Poster 2ja: Hierarchical Structuring of Biopolymers for Environmental Nanotechnologies — *Muchun Liu* 

Poster 2jb: Integrating Molecular Modeling and Machine Learning for Insight into Bulk and Interfacial Phenomena – *Alejandro Gallegos* 

Poster 2jc: Effect of PZT Loading and Surfactant Concentration on Cure Depth of PZT Ceramic Ink - Hrudaya Biswal, Janice Lucon, Cristina Stefanescu, Peter Lucon

Poster 2jd: Surface Nano-Structuring for Membranes Synthesis and Sustainable Separation Processes Development — *Yian Chen* 

Poster 2je: Permeability, Energetics and Kinetics of Photosynthetic Metabolites across Synthetic Microcompartments – Daipayan Sarkar, Christopher Maffeo, Markus Sutter, Aleksei Aksimentiev, Cheryl A. Kerfeld, Josh V. Vermaas

Poster 2jf: Computational Tools for the Discovery and Redesign of Natural and Synthetic Biological Systems – *Mohammad Mazharul Islam* 

Poster 2jg: Hybrid Materials for Clean Energy and Sustainability - Hsinhan Tsai

Poster 2jh: Computational and Experimental Study of Solvent-Based Brine Desalination. - Gabriel Barbosa

Poster 2ji: Improving Gene Therapy Manufacturing and Vector Transduction Efficiency through Capsid Engineering – *Jing Guo*  Poster 2jj: Programming Dynamic States for Directed Active Materials for Tunable Structure, Rheology, and Mechanics — *Hojin Kim* 

Poster 2jk: Sulfonated Ionomer Composite Membranes for Use in Vanadium Redox Flow Batteries - Xueting Wang, Eric M. Davis

Poster 2jl: Teaching-Focused Faculty Candidate: Using Computational Tools in Chemical Engineering Classrooms - Anukriti Shrestha

Poster 2jm: Predictive Electrolyte Thermodynamics based on openCOSMO-RS from Infinite Dilution to Ionic Liquids – *Simon Müller*, Andrés González de Castilla, Irina Smirnova

Poster 2jn: Creating a Toolbox for Studying Soft Material Self-Assembly and Dynamics - Joshua Mysona

**Poster 2jo:** Integrating Molecular Science with Systems Engineering to Drive Sustainable and Circular Economy – **Pooja Bhalode** 

Poster 2jp: Multi-Level Simulation Driven Discovery of Correlated Materials for Carbon Capture, Biomimetic Catalysis, and Quantum Information Science – Jan Niklas Boyn

Poster 2jq: High-Throughput Machine-Guided Hybrid Materials Exploration Via Combinatorial Resonant Infrared Matrix Assisted Pulsed Laser Evaporation — *Wiley Dunlap-Shohl* 

Poster 2jr: Ion and Polymer Containing Systems: From Nanoscale Physics to Engineering Applications – *Harnoor Singh Sachar* 

Poster 2js: Bring First Principles Towards Continuum: Multiscale Computational Chemistry in Fluids and Materials for Future Sustainable Energy Landscape – Rui Xu

Poster 2jt: Fundamentals of Active Transport Phenomena in Disordered Materials. — *Tingtao Zhou*  Poster 2ju: On Improving the Inadequacies in Moment Inversion Algorithm for the Extended Quadrature Method of Moments (EQMOM) – *Meltem Turan, Abhishek Dutta* 

Poster 2jv: Optimised Integrated Processes for Carbon Capture: From Direct Air Capture to Concentrated Point Sources – Marina Micari

Poster 2jw: Upcycling of Plastic Waste into Value-Added Chemicals through Oxidation and Hydrogenation Reactions - Hyunjin Moon

Poster 2jx: Monocytes Use Protrusive Forces to Generate Migration Paths in Viscoelastic Collagen-Based Extracellular Matrices – *Kolade Adebowale*, Byunghang Ha, Aashrith Saraswathibhatla, Dhiraj Indana, Medeea Popescu, Sally Demirdjian, Jin Yang, Michael Bassik, Christian Franck, Paul Bollyky, Ovijit Chaudhuri

Poster 2jy: Rational Design Strategies for Engineering Hierarchical Soft Matter - Shravan Pradeep

Poster 2jz: Toward Efficient Electricity-Powered CO<sub>2</sub> Fixation Systems with Synthetic Biology - Shanshan Luo

Poster 2ka: Unraveling the Chemistry on Metal/Metal Oxide Catalysts with Automated Mechanism Generation and Multiscale Modeling — *Bjarne Kreitz* 

Poster 2kb: Unraveling the Multi-Scale Dynamics of Soft Materials: A Path to Sustainable Engineering and Environmental Applications — *Rishabh V. More* 

Poster 2kc: Realizing the Untapped Potential of Solar-Driven Catalysis – *Aisulu Aitbekova* 

Poster 2kd: Exploring the Intersection of Heterogeneous Catalysis and Carbon Capture - Karoline Hebisch

Poster 2ke: Designer Polymers for Intracellular Organelle Engineering — Amal Narayanan Poster 2kf: Engineering of Transport Processes out of Equilibrium: Environmental Applications Driven By Fundamental Science – Fernando Temprano Coleto

Poster 2kg: Extending Automatic Reaction Mechanism Generation to Complex Systems Using Machine Learning and Computation — *Matthew S. Johnson* 

Poster 2kh: Advancing Catalyst Design through Insights from Computational Modeling - Shyama Charan Mandal

Poster 2ki: Sustainable Material Design through Machine Learning and Computer Simulations — Ludwig Schneider

Poster 2kj: Dynamic, Remote-Controllable Electroactive Hydrogel Waveguide Architectures — Oscar Alejandro Herrera Cortes Sr.

Poster 2kk: Rational Design Approaches and Engineering Effective and Stable Targeted Delivery Systems and Formulations for RNA Therapeutics – *Talia Shmool* 

Poster 2kl: Multi-Phase Ge(GeO<sub>x</sub>)/T-Nb<sub>2</sub>O<sub>5-X</sub>/C Composite with Synergistically Improved Electrochemical Performance Toward Lithium Storage — *Wei Tao, Byungchan Han* 

Poster 2km: Developing Approaches for Polymer Upcycling and Designing Sustainable Polymers – *Divya lyer* 

**Poster 2kn:** Catalyzing the Future: Creating a Confined Environment for the Production of Sustainable Chemicals — *Honghong Shi* 

Poster 2ko: Numerical Simulations of Multiphase Flows — *Ricardo Constante-Amores* 

Poster 2kp: Electrochemical Upgrading of Small Molecules Via Catalytic Microenvironment and Active Site Tuning – *Sunmoon Yu*  Poster 2kq: Modeling of Eicosanoid Class Switch during Arachidonic Acid Metabolism in Mouse Macrophage Cells Using the Cybernetic Framework – Sana Khanum, Shakti Gupta, Mano Maurya, Shankar Subramaniam, Doraiswami Ramkrishna

Poster 2ks: Direct Electrosynthesis of Ammonia from Nitrate Reduction Reaction Via Catalyst Design and Electrolyzer Engineering – *Feng-Yang Chen, Haotian Wang* 

Poster 2ku: A Systems Approach Towards Reconciling Single-Cell Heterogeneity and Cell Phenotype in Health and Disease – James Park

Poster 2kv: Electrifying the Chemical Industry Towards a Sustainable Future — *Rong Xia* 

Poster 2kw: Migrating Solvation Structures in Li-Ion Battery Electrolytes Revealed By Electrophoretic NMR – **David Halat**, Julia Im, Chao Fang, Aashutosh Mistry, Saheli Chakraborty, Darby Hickson, Venkat Srinivasan, Rui Wang, Nitash P. Balsara, Jeffrey A. Reimer

Poster 2kx: Metabolic Engineering Produce Robust Gene Therapies and Therapeutics – *Miguel Santoscoy* 

Poster 2ky: Atomic-Level Design of Sustainable Nanomaterials for Greenhouse Gas-Energy-Climate Nexus – *Haiyan (Christina) Mao* 

Poster 2kz: Exploring the Frontiers of Biotherapeutic Production: Harnessing the Power of Host Diversity, Coculture for Advancing Live Biotherapeutic Development, and Biocatalysis – *Priyanka Nain*, *Anurag Rathore, James Gomes, Aditya Kunjapur* 

**Poster 2la:** Structure-Performance Relationship of Fe-Based Catalysts for CO2 Directly Hydrogenation to Linear α-Olefins — *Chao Zhang* 

Poster 2lb: Influence of Neutral Comonomer Side Chain Length on Transport and Co-Transport of Carboxylates and Alcohols in PEGDA-Based Membranes — Antara Mazumder Poster 2Ic: Accelerating the Advancement of Functional Nanomaterials for Clean Energy Applications — **Chaochao Dun**, Jeffrey J. Urban, Mark Swihart

Poster 2ld: Catalyst Optimisation and Design for Heterogeneous Reaction Systems – *Shambhawi Shambhawi* 

**Poster 2le:** Complex Modeling in Biology: Studying Intracellular Entry in the Past and Aging in the Future – *Xinxin Wang* 

Poster 2lf: Quantifying Exosomes, Supermeres and Lipoproteins Subfractions for Early Detection of Cancer and Cardiovascular Disease — **Sonu Kumar**, John Sinclair, Nalin Maniya, Satyajyoti Senapati, Hsueh-Chia Chang

Poster 2lh: Nanoscale Thermodynamics in Liquids and Soft Materials – *Xingfei Wei* 

Poster 2li: Utilizing Microbial Communities for Valorization of Waste Carbon – **Bradley Biggs**, Manoshi Datta, Isra Raza, Markus de Raad, Hans K. Carlson, Morgan Price, Trent Northen, Adam P. Arkin

Poster 2lk: Processing-Structure-Property Relationships for Anisotropic Soft Materials - Kushal Bagchi

Poster 2ll: Meet the Candidate: Yoorae Noh – Sustainable Eco-Friendly Plastic Manufacture, Recovery, and Management – Yoorae Noh

Poster 2lm: Rapidly Ordered Block Copolymer Membranes with Tunable Pore Sizes for Wastewater Treatment — *Kshitij Sharma*, *Maninderjeet Singh, Chenhui Zhu, Mohammad Hassan, Alamgir Karim* 

Poster 2In: Redox Gel Polymer Electrolyte with Radical Molecules for Fibrous Energy Storage Devices — Jeong-Gil Kim, Jaehyoung Ko, Yongho Joo, Nam Dong Kim

Poster 2Io: Boost up the Electrical Property of CNT Fibers By Governing Impurities on the Surface of CNT with Microwave-Assisted Purification — *Min Ji Kim*, Dongju Lee, Ki-Hyun Ryu, Seo Gyun Kim, Jun Yeon Hwang, Dae-Yoon Kim, Bon-Cheol Ku, Nam Dong Kim Poster 2lp: An Optimized Miniaturized Annular Rotating Flow Reactor for Controllable Continuous Preparation of Functionalized Polysilsesquioxane Microspheres — *Tianyao Tang* 

Poster 2lq: Design of Fast-Charging Anode Interphase Based on the Understanding of Ion and Electron Transport — *Shuo Jin, Lynden A. Archer* 

Poster 2Ir: Exploring API Impregnation Technology with a Case Study on Carbamazepine — Mehrdad Khakbiz, Fernando Muzzio Sr., Gerardo Callegari

Poster 2Is: Circular Engineering Applied to Technological Processes – *Andrea Landazuri* 

Poster 2lt: Synthetic Ru/K2CO3– MgO Dual Function Materials for Integrated CO2 Capture and Conversion Via Methanation at Low Temperatures – **Tae-Young** *Kim, Jin Hyeok Woo, Jae Chang Kim, Soo Chool Lee* 

Poster 2lu: Iron-Based Catalyst for Production of Hydrogen and CNTs through the Catalytic Decomposition of Methane. – Shashank Shekhar, Kamal Pant, Shantanu Roy

Poster 2lv: Engineering and Adaptive Laboratory Evolution of *Escherichia coli* for Improving Methanol Assimilation Based on a Hybrid Xump Pathway – *Qing SUN* 

Poster 2lw: Mathematical Model of the Dezincification Behavior for the Commercial-Scale Rotary Hearth Furnace – Jinsu Kim, Moon-Kyung Cho, Myungwon Jung, Jeeeun Kim, Young-Seek Yoon

Poster 2lx: Meet the Post-Doc Candidates Session: Process Intensification for Industrial Crystallizations Via Process Control and Design Strategies – Montgomery Smith

Poster 2ly: Energy and Charge Transport and Forces in Novel Chemical Environments - Mohammadhasan Dinpajooh

Poster 2lz: Spatial Systems Biology for Translational Cancer Immunotherapy — *Alexander Xu*  Poster 2ma: Integrating Simulations and Experiments to Elucidate Ion and Small Molecule Transport in Polymeric Materials – Everett Zofchak

Poster 2mb: Programmable Synthetic Circuits for Smart Therapeutics — *Alexander Vlahos* 

Poster 2mc: Engineering and stabilizing cell aggregates for synthetic multicellularity – *Heidi Klumpe* 

Poster 2md: Conjugated polymers based bioelectronic sensors for living-nonliving interfaces - Sujitkumar Bontapalle

Poster 2me: Utilizing Computational Methods for the Design and Enhancement of Energy Storage Systems – *Yiling Nan* 

Poster 2mf: Machine-Learning Driven Exploration of Catalytic Reaction Networks — *Hyunwook Jung* 

**Poster 2mg:** Transforming cell therapy manufacturing and cancer management with large-volume microfluidics – *Avanish Mishra* 

Poster 2mh: Empowering Health through Engineering: Utilization of Drug Delivery and Nanotechnology Towards Improved Health Equity - Olivia Lanier

Poster 2mi: Advancing Switchable Solvents for the Sustainable Water Reuse and Desalination Applications – *Kinnari Shah* 

Poster 2mj: Extending a Microfluidic Platform to Elucidate Bacterial Communication in humans its impact on disease - Corine Jackman Burden

Poster 2mk: Electrochemistry Nano Laboratory (Echem NanoLab): Wearable sensing platforms for continuous health monitoring — *Farnaz Lorestani* 

Poster 2ml: Creating Advanced Therapeutics and Applications in Enzyme-Controlled Spatiotemporal Technologies – *Zhimin Huang*, *Jerzy Szablowski*  Poster 2mm: Interfacial Engineering for Plasmon-Enhanced Nanomaterials for Energy Conversion and Biosensing applications – *Lemma Tufa, Jaebeom Lee* 

Poster 2mn: Cell-Free Synthetic Biology by Design for Precision Medicine – Yan Zhang

Poster 2mo: Design of Advanced Functional Materials for Cardiovascular engineering — *Renato Navarro* 

Poster 2mp: Bio- and Art-inspired Bioelectronics for Next-generation Brain-machine Interface — *Xiao Yang* 

Poster 2mq: 2D Materials for Applications in Optoelectronics, Energy Harvesting and Beyond — Debjit Ghoshal

Poster 2mr: Multiscale Modelling Framework to Understand the Effect of Site Heterogeneity on Activity in Paramagnetic Single Atom Catalysts — *Sanjana Srinivas* 

(3) Area Plenary: Bionanotechnology (Invited Talks)

Sunday, Nov 5, 3:30 PM Hyatt Regency Orlando, Bayhill 29

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

Sponsored by: Bionanotechnology

**3:30 Paper 3a:** Micro/Nanoengineered Adhesive Biomaterials for Regenerative Medicine and Drug Delivery — *Nasim Annabi* 

**4:20 Paper 3b:** Harnessing Chaos: Rational Design of Nanoscale Surfaces for Cavitation-Based Imaging Agents, Nanomotors, and Protein Therapeutics. – *Andrew Goodwin* 

5:10 Paper 3c: Building Bioactivity and Nanostructure into Slippery Liquid-Infused Porous Surfaces — David M. Lynn (4) 3D Printing Fundamentals and Applications

Sunday, Nov 5, 3:30 PM Hyatt Regency Orlando, Bayhill 33

William Phillip, Chair Monirosadat Sadati, Co-Chair

**Sponsored by:** 3D Printing and Advanced Manufacturing

3:30 Paper 4a: Additive Manufacturing of Functional Medical Devices for Use in the Clinic – Matthew Becker

**4:00** Paper 4b: Single and Multiphase Flows in Well-Defined Periodic 3D-Printed Lattices — *Ian Woodward, Yinkui Yu,* Catherine Fromen

**4:30** Paper 4c: Printing 3D Structures with Controlled Chiral Self-Assembly — *Mohsen Esmaeili, Kyle George, Nader Taheri-Qazvini, Monirosadat Sadati* 

4:48 Paper 4d: Developing Blood-Mimicking Fluid Formulations to Match Refractive Index of Compliant SLA 3D-Printed Vascular Model – *Elnaz Hosseinzadeh*, Beatriz Alejandra Bosques Palomo, José Antonio Lorenzo Oliver, Alan Aguirre Soto

5:06 Paper 4e: Multi-Order Combinatorial Lattices for Spatial Control of Transport Phenomena — Ian Woodward, Catherine Fromen

5:24 Paper 4f: A Novel Means of Measuring Key Thermphyscal Properties Needed for Additive Manufacturing in Space – Jason Livesay, Ranga Narayanan, Robert Singiser, Zachary Karpinski, Linnea Helenius, Joshua Fosen

5:42 Paper 4g: Fundamental Study on Processing-Structure-Properties Relationships of Acrylonitrile-Butadiene-Styrene (ABS) for Material Extrusion Additive Manufacturing (MatEx AM) – Juhyeong Lee, Jay Park (5) New Faculty Forum (Invited Talks)

Monday, Nov 6, 8:00 AM Hyatt Regency Orlando, Bayhill 30

Jerrod Henderson, Chair Marissa Wechsler, Co-Chair

**Sponsored by:** Young Faculty Forum

8:00 Paper 5a: Becoming an Assistant Professor — *Sophia Orbach* 

8:25 Paper 5b: Transition in Progress – Damilola Daramola

8:50 Paper 5c: Learning on the Job: Launching an Academic Career — *Karthish Manthiram* 

9:15 Paper 5d: Making Your Research Matter: Strategies for Successful Broader Impacts Statements – *Sindia M. Rivera-Jimenez, Sarah Wilson* 

9:55: Panel Discussion

#### (6) High Pressure Phase Equilibria and Modeling

Monday, Nov 6, 8:00 AM Hyatt Regency Orlando, Orlando Ballroom M

Aaron Rowane, Chair Steven Saunders, Co-Chair

Sponsored by: High Pressure

8:00 Paper 6a: Phase Behaviour of Isobutane + CO<sub>2</sub> and Isobutane + H<sub>2</sub> at Temperatures between 190 and 400 K and at Pressures up to 20 MPa – *Riley Latcham, Martin Trusler* 

8:20 Paper 6b: Application of a Synthetic Method for Calculations of Solubilities and Diffusion Coefficients of Carbon Dioxide and Nitrogen in Polystyrene – *Hossein Abedsoltan* 

8:40 Paper 6c: Evaluating the Effect of Water Fractions on Methane Hydrate Formation and Inhibition Performance of Amino Acid L-Proline in Gas-Dominated System for Offshore Flow Assurance. – *M Fahed Qureshi, Majeda Khraisheh*  **9:00 Paper 6d:** Solubility of Light Gases in Water and NaCl Brines at High Pressures – **Qiaoyun Chen**, *Geraldine A. Torin-Ollarves, Martin Trusler* 

9:20 Paper 6e: Phase Behavior of H<sub>2</sub>+Gas+Brine Systems and H<sub>2</sub> Dissolution Kinetics Under Subsurface Storage Conditions: Experiments and Thermodynamic Modeling – Salaheddine Chabab, Halla Kerkache, Marie Poulain, Guillaume Galliero, Pierre Cezac

**9:40 Paper 6f:** The Effects of Polymeric Additives on the High-Pressure Thermodynamic and Rheological Properties of Mineral Lubricant Base Oils – *Katrina Avery, Erdogan Kiran, Mark Devlin, John C. Hassler* 

**10:00 Paper 6g:** Development of a Custom High-Temperature, High-Pressure Phase Behavior Apparatus — *Aaron Rowane* 

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

Monday, Nov 6, 8:00 AM Hyatt Regency Orlando, Plaza International Ballroom I

Shikha Nangia, Chair Sumit Sharma, Co-Chair

**Sponsored by:** Thermodynamics and Transport Properties

8:00 Paper 7a: Accomplishments, challenges and outlook for accelerating and optimizing materials and processing discovery using machine learning - Paulette Clancy

8:30 Paper 7b: Applications of Machine Learning and Bayesian Statistics in Coarse-Grained Molecular Dynamics — Sanket Deshmukh

**9:00 Paper 7c:** Coarse-grained simulations of side chain liquid crystal polymers with different types of attachments – *Diego Becerra*, *Lisa Hall* 

9:30 Paper 7d: Achieving Quantum Mechanical Accuracy for Modeling Reaction-diffusion Process in Liquid-phase Heterogeneous Catalysis - Neeraj Rai (8) Environmental Division Awards and Honors (Invited Talks)

Monday, Nov 6, 8:00 AM Hyatt Regency Orlando, Blue Spring I/II

Kerry Kelly, Chair Alexander Orlov, Co-Chair

**Sponsored by:** Environmental Division

8:00 Paper 8a: Lowering the Barriers to Clean Water through Catalysis — *Michael Wong* 

8:45 Paper : Electrochemical Wastewater Refining: Reactive Separations to Convert Pollutants into Products – *William Tarpeh* 

(9) Environmentally Friendly Product and Process Development for Sustainability

Monday, Nov 6, 8:00 AM Hyatt Regency Orlando, Bayhill 28

Jing Luo, Chair Kakasaheb Nandiwale, Co-Chair Madhav Ghanta, Co-Chair

Sponsored by: Process Research and Innovation

8:00 Paper 9a: Development and Optimization of a Continuous API Manufacturing Process — Cameron Armstrong, Katharina Grohowalski, Kakasaheb Y. Nandiwale, David Bernhardson, Pablo Jose Cabrera Ventura, Sergei Tcyrulnikov, Alexander Hesketh, David Limburg, Steven M. Guinness

8:25 Paper 9b: Composition-Property Relationships of BP-1 Lunar Regolith Binders for in-Situ Resource Utilization As Geopolymers & *Planetopolymers* – Thaddeus Egnaczyk, Quent Hartt, Jennifer Mills, Norman J. Wagner

8:50 Paper 9c: Sustainable Manufacturing and Life Cycle Assessment of MOF-Polymer Composites By Reactive Extrusion – Yufeng Quan, Harold Escobar Hernandez, Qingsheng Wang

9:15 Paper 9d: Demonstration of a Sustainable Pathway for Producing Fully Bio-Based Polyethylene Terephthalate (bio-PET) — Parikshit Sarda, Sridhar Viamajala, Joseph Lawrence 9:40 Paper 9e: Sustainable One-Pot Production of Diformylxylose from Agricultural Biomass: Process Development, Scaling-up, and Life-Cycle Assessment – Anastasiia Komarova, Zezhong Li, Jeremy Luterbacher

**10:05 Paper 9f:** Selection of Greener Solvents Using Computer-Aided Molecular Design (CAMD) to Extract Octacosanol from Filter Press Mud of Sugarcane - *Nistala Venkata* 

**Subrahmanyam**, Sharad Bhartiya, Urmila Diwekar

(10) Regenerative Engineering Society

Monday, Nov 6, 8:00 AM Hyatt Regency Orlando, Regency Ballroom P

Johnna Temenoff, Co-Chair Yupeng Chen, Co-Chair

**Sponsored by:** Regenerative Engineering Society

8:00: Introductory Remarks

8:20 Paper 10a: Delivery of Biologics for Muscle Healing after Rotator Cuff Injury – Johnna Temenoff

8:50 Paper 10b: Bioengineered perfused human brain microvasculature for brain tumor and neural stem cell research - Guohao Dai

**9:20 Paper 10c:** Tailoring Intelligent Protein Engineered Biomaterials for Regenerative Medicine — *Jin Kim Montclare* 

9:50 Paper 10d: Engineer Off-the-Shelf CAR-Neutrophils for Targeted Chemoimmunotherapy Against Glioma – *Xiaoping Bao* 

10:10 Paper 10e: Immunobioengineering of a Three-Dimensional Polymeric Scaffold-Based Implantable Thymic Organoid – *Manpreet Bariana*, *Elena Cassella, Shaina Anuncio, Jakub Erben, Andrea Tuckett, Michael Poulos, Jason Butler, Johannes Zakrzewski*  (11) Division Plenary: Gerhold and Kunesh Awards on Separations (Invited Talks)

Monday, Nov 6, 8:00 AM Hyatt Regency Orlando, Barrel Spring I

Seth Huggins, Chair Isaac Gamwo, Co-Chair Marina Tsianou, Co-Chair

**Sponsored by:** Separations Division

8:00: Welcoming Remarks

8:05 Paper 11a: Fundamental Membrane Science Research Addressing the Water-Energy Nexus — *Benny D. Freeman* 

8:32 Paper 11b: Purification of Circular RNA By Ultrafiltration - Scott Husson

8:59 Paper 11c: Polymer Membranes with Engineered Microporosity for Gas Separations - *Ruilan Guo* 

**9:26 Paper 11d:** Redox-Mediated Electrochemical Separations: From Fundamentals to Applications — *Xiao Su* 

**9:53 Paper 11e:** Development of Membrane Based Operations for Emerging Separations Challenges — *Ranil Wickramasinghe* 

10:20: Concluding Remarks

(12) Sustainable Pathways to Clean Hydrogen and Synthetic Fuels I

Monday, Nov 6, 8:00 AM Hyatt Regency Orlando, Columbia 36

William Gibbons, Chair Eric Miller, Co-Chair

**Sponsored by:** Sustainable Pathways Toward Hydrogen and Synthetic Fuels

8:00 Paper 12a: US Department of Energy Hydrogen Program Overview — *Eric Miller, William Gibbons*  8:25 Paper 12b: H2NEW Lab Consortium: Increasing the Performance and Durability of Electrolysis for Clean, Competitive Production of Hydrogen — Richard Boardman, Bryan S. Pivovar, David Peterson, William Gibbons, Mark Ruth, Daniel Wendt, Olga Marina, Rangachary Mukundan

8:50 Paper 12c: Doe Thermal Conversion with Carbon Capture and Storage R&D – *Eva Rodezno* 

**9:15 Paper 12d:** U.S. Doe Overview - Supporting Clean Hydrogen through Supply Chain and Recycling Research and Development Efforts – *Julie Fornaciari* 

**9:40 Paper 12e:** Renewable to Liquid Fuels Beyond the Grid – *James Seaba* 

(13) MAC Eminent Engineers Awards Poster Session

Monday, Nov 6, 11:00 AM Hyatt Regency Orlando, Regency Ballroom R/S

Ingrid J. Paredes, Co-Chair Deisy Cristina Carvalho Fernandes, Co-Chair Jorge Almodovar, Co-Chair

**Sponsored by:** Minority Affairs Community (MAC)

Poster : Assessing the Production and Cytocompatibility of *Plodia Interpunctella* silks as Polymeric Biomaterials – **Jasmine McTyer**, Bryce Shirk, Lauren Eccles, Isabella Torres-Duarte, Andrea Orozco, Paul Shirk, Whitney Stoppel

Poster : Assessing the Feasibility of Coal As an Eco-Friendly Filler in Phenolic Resin Composites: A Study of Thermal and Structural Properties — *Chiderah Chukwuka*, *Damilola Daramola*, *Sophia Almanza* 

Poster : Exploring the Economic and Environmental Benefits of Solvent-Based Recycling Processes of Multi-Layer Plastic Films — *Aurora Del Carmen Munguia Lopez*, Dilara Goreke, Kevin Sanchez-Rivera, Horacio Aguirre-Villegas, Styliani Avraamidou, George Huber, Victor Zavala Poster : Confirming the Extent and Mechanisms of the Immunosuppressive Enhancement of hMSCs Initiated By Col/Hep Layer By Layer Polyelectrolyte Coatings – Justin Putman, Roaa Hadi, Jorge Almodovar

Poster : Unraveling the Enhancing Effect in Proliferation of Human Mesenchymal Stem Cells Cultured on Biopolymeric Coatings. — **Roaa Hadi**, Jorge Almodovar, Justin Putman, Luis Carlos Pinzon-Herrera

**Poster :** Exploring the Impact of Coinfections Involving Epstein-Barr Virus (EBV) and Malaria on the Development of Autoimmune Diseases in Patients. — *Charlene Chung* 

Poster : Enhancing Magnetic Particle Imaging (MPI) Performance: Probing Post-Synthesis Oxidation and Correlations to Nanoparticle Properties — *Ambar Velazquez Albino*, *Aniela Nozka*, *Andrii Melnyk*, *Hayden Good*, *Carlos Rinaldi-Ramos* 

Poster : Electrified Lixiviation of Rare Earth Elements from Coal Mining Waste - MAC – *Lawrence Ajayi*, *Damilola Daramola* 

Poster : Extraction and Characterization of Cellulose Nanocrocrystals from Corn Husk Waste and Its Application in Bioplastic Preparation — Sergio Mayta Paucara, Maria Quintana Caceda, Ronny G. Huamani Palomino, Bryan M. Córdova

Poster : Demonstration of a Batch Electrochemical System for Phosphorus Recovery from a Real Municipal Wastewater Recycle Stream - MAC Session — **Sana Heydarian**, Syed Asad Abbas, Lawrence Ajayi, Jason Trembly, Damilola Daramola

Poster : Hydrophobic Collapse of Long Alkane Chains in Water and Water/Ethanol Mixtures — **Rahul Kumar**, David Abadie, Nicole Korinetz, Henry Ashbaugh

Poster : MAC Poster: Mathematical Modeling of Drug Release from Bi-Layered Drug Delivery Systems in the Eye – Eduardo A. Chacin Ruiz, Jabia M. Chowdhury, Katelyn E. Swindle-Reilly, Ashlee N. Ford Versypt Poster : Biorefrineries for a Sustainable Plastic Value Chain — *Efrain Rodriguez-Ocasio, Mark Blenner, Laura R. Jarboe* 

Poster : Tri-Component Microneedle Patch for Enhanced Veterinary Meloxicam Delivery: PVA, Collagen, and Chitosan Synergies – Jorge Almodovar

Poster : Dielectrophoresis-Based Breast Cancer Study: Characterization and Separation of Peripheral Blood Mononuclear Cells from Pymt and WT Mouse Model — Raphael Oladokun, Christopher Smith, Timothy Eubank, Soumya Srivastava

#### (14) Featured MPC Session: Sustainability and the Circular Economy Panel Discussion

Monday, Nov 6, 11:00 AM Hyatt Regency Orlando, Plaza International Ballroom G/H

Yu Shi, Chair Martha Grover, Co-Chair

Sponsored by: Miscellaneous

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

Monday, Nov 6, 12:30 PM Hyatt Regency Orlando, Bayhill 23

Fani Boukouvala, Chair Chrysanthos Gounaris, Co-Chair

**Sponsored by:** Computing Systems and Technology Division

12:30 Paper 15a: Designing a Sustainable Supply Chain for Polyolefins Waste Management: A Multi-Objective Optimization Approach — Oluwadare Badejo, Borja Hernández Blázquez, Marianthi Ierapetritou

12:45 Paper 15b: A Bayesian Optimization Framework for Interconnected Systems – Leonardo Gonzalez, Victor Zavala

**1:00** Paper 15c: Inverse Mixed-Integer Optimization for Learning Interpretable Decision Rules — *Rishabh Gupta, JOHN Wassick, Qi Zhang*  **1:15 Paper 15d:** Efficient Numerical Strategies for Multidimensional Population Balance Models and Transport Equations – **Pavan Inguva**, Francesco Destro, Richard Braatz

**1:30 Paper 15e:** Accelerating Drug Discovery and Development Using an Ontology-Based Machine Learning Framework — *Vipul Mann*, Shekhar Viswanath, Shankar Vaidyaraman, Venkat Venkatasubramanian

1:45 Paper 15f: Taking the Human out of the Decomposition-Based Optimization Loop Via Artificial Intelligence and Network Science – *Ilias Mitrai, Prodromos* Daoutidis

2:00 Paper 159: Enabling Cyberattack Detection in Process Control Systems Via Randomized Controller Switching – *Shilpa Narasimhan, Nael El-Farra, Matthew Ellis* 

2:15 Paper 15h: High-Dimensional Bayesian Optimization of Molecular Properties Using Quantitative Structure-Property Relationships on Sparse Axis-Aligned Subspaces — Farshud Sorourifar, Thomas Banker, Joel Paulson

(16) Introduction to NSF's CBET Division and Proposal Writing Strategies

Monday, Nov 6, 12:30 PM Hyatt Regency Orlando, Bayhill 29

Carole Read, Chair Ram Gupta, Co-Chair

**Sponsored by:** Career Guidance Committee Liaison

**12:30 Paper 16a:** Division Director Update on the Chemical, Bioengineering, Environmental, and Transport Systems Division of NSF: Programs and Opportunities – *Jeanne VanBriesen* 

1:20 Paper 16b: Proposal Writing Strategies for Fundamental Research Proposals for NSF - Gregory L. Rorrer (17) Plenary Session on Novel Flows (Invited Talks)

Monday, Nov 6, 12:30 PM Hyatt Regency Orlando, Plaza International Ballroom K

#### Simon Rogers, Chair

Sponsored by: Fluid Mechanics

**12:30 Paper 17a:** The Role of Rolling Resistance in the Rheology of Wizarding Quidditch Ball Suspensions – **Sarah Hormozi**, Donald L. Koch, Enzo d'Ambrosio

**1:05** Paper 17b: Influence of Charge Fraction and Sequence on Polyelectrolyte Solution and Brush Properties – *Amanda B. Marciel* 

1:40 Paper 17c: Tailoring Anisotropic Nanomaterial Liquid Crystal Dispersions: From Fiber Spinning to Direct Ink Writing – Virginia Davis

2:15 Paper 17d: Rheological Characterization and Design of Highly-Filled Inks for Direct-Ink Write Additive Manufacturing — Jessica Kopatz, Derek Reinholtz, James Griebler, Jonathan Leonard, Alexander Tappan, Adam Cook, Anne Grillet

(18) Design and Analysis of Carbon Capture and Negative Emissions Technologies -Experimental

Monday, Nov 6, 12:30 PM Hyatt Regency Orlando, Blue Spring I/II

Dora Lopez De Alonzo, Chair Omar Guerra, Co-Chair Toufiq Reza, Co-Chair Monday Okoronkwo, Co-Chair

Sponsored by: Climate Change

**12:30 Paper 18a:** Screening of lonic Liquids for CO<sub>2</sub> Capture at Ambient Conditions – *Rohit Chauhan*, *Rohan Sartape*, *Meenesh R Singh* 

12:47 Paper 18b: Controlled Morphology, Post-Synthetic Modification, and Scale-up of MOFs for Direct Air Capture of Carbon Dioxide — Xakin Ramirez Isunza, Brittany Bonnett, Connor Farrell, Amanda J. Morris, Stephen Martin **1:04 Paper 18c:** Energy-Efficient and Stable Amine Structures Supported By Mesoporous Silica for Direct Air Capture — *Joo-Youp Lee, Soumitra Payra* 

1:21 Paper 18d: CO<sub>2</sub> Capture Using Phase-Changing Bis-Iminoguanidines (BIGs) with Amino Acids; Analysis of a Direct Air Capture Process — *Abishek Kasturi*, Gyoung Gug Jang, Diana Stamberga, Radu Custelcean, Sotira Yiacoumi, Costas Tsouris

**1:38** Paper 18e: Investigating Oxidative Degradation Products and Mechanisms of Aminopolymer Sorbents for Direct Air Capture (DAC) – **Yoseph Guta**, Tianchang (Athena) Xu, Juliana Carneiro, Giada Innocenti, Simon H. Pang, Miles Sakwa-Novak, Nga Lee Ng, Carsten Sievers, Christopher Jones

**1:55 Paper 18f:** Direct Air Capture with Amino Acid Solvent: Operational Optimization Using a Crossflow Air-Liquid Contactor - *Keju An* 

2:12 Paper 18g: Amino Acid-Based Functionalized Deep Eutetuc Solvents As a Promising Alternative for Efficient CO<sub>2</sub> Capture and Consideration of Its Application — Jaehan Jo, Minseok Park, Seokho Kwon, Dongwoo Kang

2:29 Paper 18h: Ultra-Functional CO<sub>2</sub> Capture Sorbent Development Via One-Pot Deep Eutectic Solvent Based Thermochemical Conversion — Al Ibtida Sultana, Md Tahmid Islam, Josh Calhoun, Robert Cheatham, Toufig Reza

**2:46:** Carbon Capture Networking and Informing New Sessions in the AIChE ENV Division

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

Monday, Nov 6, 12:30 PM Hyatt Regency Orlando, Celebration 9

Matthew Webber, Chair Amol Janorkar, Co-Chair Yifan Cheng, Co-Chair

# Sponsored by: Biomaterials

**12:30 Paper 19a:** Recent Advances in Zwitterionic Materials for Biomedical and Engineering Applications – *Shaoyi Jiang*  **1:20 Paper 19b:** Multiscale Control of Biomaterials for Engineered Extracellular Matrices – *Adrianne Rosales* 

2:10 Paper 19c: Rational Design of Antifouling Topographies to Control Biomaterial-Associated Infections – *Dacheng Ren* 

(20) Advances in Fluid Particle Separations

Monday, Nov 6, 12:30 PM Hyatt Regency Orlando, Barrel Spring II

Jenifer Gomez Pastora, Chair Seyi Odueyungbo, Co-Chair

**Sponsored by:** Fluid-Particle Separations

12:30 Paper 20a: Development of Electrospun PCL Aerosol Filter Media for Respiratory PPE Applications – Nathan Ewell, Gregory Rutledge

12:55 Paper 20b: Refinement of the Relationship between Brownian Force and Magnetic Force on Superparamagnetic Iron Oxide Nanoparticles – *Xian Wu*, *Hyeon Choe, Jacob Strayer, Jenifer Gomez Pastora, Barbara E. Wyslouzil, Jeffrey Chalmers* 

**1:20** Paper 20c: Dynamic Modeling of Solid Bowl Centrifuges As a Tool for Better Process Design: Advantages of Adaptive Hybrid Models – *Marco Gleiss* 

1:45 Paper 20d: Development of Regenerable Fine Particulate Air Filters – Andrew L. Wagner, Matthew Emmons, Matthew Haggerty

2:10 Paper 20e: Effect of a Recirculation System in an Industrial Cyclone Separator – Praveen Kumar Nedumaran, Praveen Kumar Nedumaran, Dzmitry Misiulia, Sergiy Antonyuk

(21) Area Plenary: Adsorption and Ion Exchange - In Honor of Prof James A Ritter (Invited Talks)

Monday, Nov 6, 12:30 PM Hyatt Regency Orlando, Manatee Spring I

F Handan Tezel, Chair Daniel Siderius, Co-Chair

**Sponsored by:** Adsorption and Ion Exchange

(22) Honorary Session for Prof. Rich Noble

Monday, Nov 6, 12:30 PM Hyatt Regency Orlando, Barrel Spring I

Alexander Lopez, Chair Jason Bara, Co-Chair Isabel Escobar, Co-Chair

**Sponsored by:** Membrane-Based Separations

**12:30 Paper 22a:** Development of a Membrane Process to Capture CO2 Emissions from Industrial Processes. — *Richard Baker* 

**1:00 Paper 22b:** Sterile Filtration of mRNA-Lipid Nanoparticle Vaccines – New Challenges for an Old Technology – *Andrew Zydney* 

**1:30** Paper 22c: Prof Rich Noble and the Membrane Science, Engineering and Technology Center – *Ranil Wickramasinghe* 

**2:00** Paper 22d: Transformational Membranes for Carbon Capture and Utilization — **Shiguang Li**, *Miao Yu, Xinhua Liang, Fan Wang, Dinesh Behera, Qiaobei Dong, Weiwei Xu, Howard Meyer* 

**2:30** Paper 22f: Electrochemically facilitated transport of CO<sub>2</sub> between gas diffusion electrodes in flat and hollow fiber geometries – *Kyle M. Diederichsen,* Younghun Lee, Michael Massen-Hane, **T Alan Hatton** 

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

Monday, Nov 6, 12:30 PM Hyatt Regency Orlando, Manatee Spring II

Christopher Burcham, Chair Gerard Capellades, Co-Chair

**Sponsored by:** Crystallization and Evaporation

12:30: Welcoming Remarks

**12:35 Paper 23f:** Solid-State Deracemization of Conglomerate-Forming Chiral Compounds, Simple and Ubiquitous – *Marco Mazzotti* 

1:20: Discussion

1:30 Paper 23a: Creatine Citric Acid Cocrystals or Creatine Citrate Salts, That Is the Question? — Greg York

**1:48 Paper 23b:** Optimization of a Commercial-Scale Agrochemical Crystallization Prone to Oiling and Agglomeration — **Paul Larsen**, Zoltan Benko, Venkateswarlu Bhamidi, Jay Bradstreet II, Steve Coats, Navraj Hanspal, Yamini Krishnan, Ipsita Mishra, Kevin Peil, Xi Yang

2:06 Paper 23c: Opencrystaldata: An Open-Access Crystal Image Database for Enabling the Image-Based Analysis of Crystallization Systems – Wei-Lee Wu, Yash Barhate, Christopher Boyle, Hossein Salami, Andreas Bommarius, Javier Cardona, Zoltan Nagy, Ronald Rousseau, Martha Grover

2:24 Paper 23e: Microfluidic Phase Diagram of Sucrose Droplets: Freezing, Freeze-Concentrated Glass Transition, and Melting Temperatures — *Leif-Thore Deck*, **Nadia Shardt**, Imad *El-Bakouri, Florin N. Isenrich, Andrew J. deMello, Ulrike Lohmann, Marco Mazzotti* 

2:42 Paper 23d: 'Regeneration' Phenomenon Observed in Pharmaceutical Crystals Post Breakage – a Case Study on Paracetamol and the Effect of Growth Solvents – Isha Bade, Vivek Verma, Allison Arber, Jerry Heng

(24) Materials Interfaces -Celebrating the Career of John Ekerdt

Monday, Nov 6, 12:30 PM Hyatt Regency Orlando, Celebration 10

Jane Chang, Chair Gyeong Hwang, Co-Chair

**Sponsored by:** Material Interfaces as Energy Solutions

**12:30 Paper 24a:** Chemical Processing of Function Accelerated Nano-Materials at the Atomic Scale – *Jane Chang* 

12:48 Paper 24b: Surface Reaction Kinetics during Area-Selective Thin Film Deposition — Gregory N. Parsons **1:06 Paper 24c:** Controlling Nucleation and Selectivity in Atomic Layer Deposition for Materials Synthesis – *Stacey Bent* 

**1:24 Paper 24d:** High Quality Tunable Plasmonic Nanostructures By Atomic Layer Deposition — *Brian Willis*, John A. Grasso, Rahul Raman

1:42 Paper 24e: Chemical "Engineerifying" Electronics — *Michael A. Filler* 

2:00 Paper 24f: The Elusive Surface M2O7 Dimer Active Site — Israel Wachs

2:18 Paper 24g: The Dual Nature of Chemical Reaction Engineering - James Rawlings

2:36 Paper 24h: Plasma Enhanced Atomic Layer Deposition of Silicon Carbonitride — Samuel Johnson, Tsung-Hsuan Yang, Jianping Zhao, Toshihiko Iwao, Charles Schlechte, John Carroll, Gabriel Blankemeyer, Peter Ventzek, Joaquin Resasco, Gyeong S. Hwang, John Ekerdt

## (25) Graduate Education and Support

Monday, Nov 6, 3:30 PM Hyatt Regency Orlando, Bayhill 28

Adam Melvin, Chair Mo Jiang, Co-Chair Weijian Diao, Co-Chair

# **Sponsored by:** Graduate Education

**3:30** Paper 25a: Perspective on Starting a Mentoring Program for First Year Ph.D. Students - Mariah Arral

**3:45 Paper 25b:** Teaching Chem-E Journal Club: An Opportunity for Career Exploration and Student Support — *Rebecca Harmon* 

**4:00** Paper 25c: Green Chemical Engineering Innovation: Turning Design Constraints into a Source of Creativity – *Christopher V. H-H. Chen* 

**4:15 Paper 25d:** Retrospective Analysis of the Effect of an Online "Bridging" Course Sequence on Student Success in Graduate Studies – *Matthew Cooper, Lisa Bullard, Aaron Frye*  (26) IDEAL Featured Session: A Conversation on Equity, Diversity, and Inclusion

Monday, Nov 6, 3:30 PM Hyatt Regency Orlando, Plaza International Ballroom G/H

Martha Grover, Chair Lori McDowell, Co-Chair Yu Shi, Co-Chair Christopher Pope, Co-Chair

**Sponsored by:** Engineering for Inclusion

# (27) Poster session: Bioengineering

Monday, Nov 6, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

Jamie Spangler, Chair Yongchan Kwon, Co-Chair Christopher Kieslich, Co-Chair Jason Boock, Co-Chair Phanourios Tamamis, Co-Chair

Sponsored by: Bioengineering

# BIOCATALYSIS AND BIOBASED PRODUCTS

Poster 27a: Photoenzymatic Asymmetric Hydroamination of Simple Aliphatic Amines and Vinyl Arene Olefins — *Wesley Harrison, Huimin Zhao* 

Poster 27c: Understanding and Engineering Chain Translocation in Assembly-Line Polyketide Synthases – *Alexander Soohoo*, *Dillon Cogan, Chaitan Khosla* 

Poster 27d: Polyethylene Terephthalate (PET) Plastic Intermediates Deconstruction in One Pot *B. Subtilis* Bioprocess — *Apurv Mhatre*, Bethany Kalsheur, Haley McKeown, Bruce Rittmann, Arul Mozhy Varman

Poster 27e: Cellulose Hydrolysis Using Chitosan Coated Enzyme-Magnetic Nanoparticle – *Heejoon Park* 

Poster 27f: Process Development and Techno-Economic Analysis of Biomass-Derived GVL Production As an Intermediate for Chemo-Enzymatic Bio-Jet Fuel Production – Joungho Park, Kyung-Ran Hwang, Kyoungseon Min Poster 27g: Polymer Motion Energizing Enzyme Conformational Dynamics and Catalytic Kinetics in Organic Solvents – Yupei Jian, Zheng Liu

Poster 27h: Simulation-Based Evaluation of the Pre-Treatment of Acid Raw Materials in Biodiesel Production — Francisco Lucas Carneiro, Marcilio Maximo, Bianca Viana, Fernando V. Lima, Heleno Bispo

Poster 27i: Improving Biomass-Derived Graphene Coating on Transitional Metals — *Suriya Narayanan Ramasubramanian, Hema Ramsurn, Gabriel LeBlanc* 

Poster 27j: Impact of pH Adjustment on Hydrogen Production in Pressurized Gas Fermentation — *Gwon Woo Park, Myounghoon Moon, Min-Sik Kim* 

Poster 27k: Development of a Cell Culture-Derived Viral Insecticide to Control the Spread of *Drosophila Suzukii — Keven Lothert, Yasmina Harsy, Thorsten Gröb, Kwang-Zin Lee, Michael W. Wolff* 

## CELL CULTURE ENGINEERING AND BIOPHARMACEUTICAL MANUFACTURING

Poster 27m: Bioreactors Scale-up and Optimization from Lab to Manufacturing Scale — *Nima Yazdanpanah* 

Poster 27n: Fluorescence Complementation Enables Quantitative Imaging of Transcription Factor Delivery in Plants – *Henry Squire*, *Jeffrey Wang, Natalie S. Goh, Heyuan M. Ni, Edward Lien, Cerise Wong, Eduardo Gonzalez-Grandio, Markita Landry* 

Poster 270: Effect of Oxidative Stress on Pertactin Productivity in *Bordetella Pertussis* Fermentations: A Study on Glutamate-Induced ROS Inhibition – Abhishek Mishra, Melih Tamer, Hector M. Budman

# PROTEIN SCIENCE AND ENGINEERING

Poster 27q: Probing the Origins of Collateral Fitness Effects of Mutations – *Cameron Goff, Marc Ostermeier*  Poster 27r: Enhanced Protein Stability Enabled By Mixtures of Ionic and Amphoteric Surfactants Compared to Each Alone — Tridwip Sen, Evan Danielson, Kerri Peterson, Kayla Thompson, Elaine Reece, Jason Berberich, Jason Boock

Poster 27s: Adaptability of 22 Functional Cas12a Orthologs Using a Combinatorial Approach for Nucleic Acid Detection in Clinical Samples – *Dylan Carman, Long Nguyen, Noah Rakestraw, Nicolas C. Macaluso, Piyush Jain* 

Poster 27t: Comparison of GST and SUMO Fusion Tags for Enhanced Yield and Purity of Recombinant Osh4 – *Andrew Loveland*, *Dinara Konakbayeva*, *Jeffery Klauda, Amy Karlsson* 

Poster 27u: Understanding the Inherent Bias in the Activity of Mismatch Specific Exonuclease - Rushant Sabnis, Qing Sun

Poster 27v: Engineering Bispecific Receptor Decoy Antagonists to Treat Neovascular Eye Diseases — *Emily Ariail, Paul Sargunas, Jamie Spangler* 

**Poster 27w:** Metabolic Engineered *Escherichia coli* Strains to Express Flavoprotein Monooxygenases from Actinomycetes Isolated from the Atacama Desert for Industrial Applications. — *Carolina Gonzalez, Irene Martinez* 

Poster 27x: Computational Design of Peptides As Detectors, Drugs, and Biomaterials – *Sudeep Sarma*, Greg Hudalla, Stefano Menegatti, Nathan Crook, Scott Magness, Anant Paravastu, Carol Hall

Poster 27y: Characterizing Cas12i Proteins As Novel Enzymes for Diagnostics and Gene Editing – Carlos Orosco, Santosh Rananaware, Minji Chang, Zoe Fang, Lilia Yang, Noah Rakestraw, Grace Shoemaker, Katelyn Meister, Jordan Lewis, Briana Pizzano, Piyush Jain

Poster 27z: Assessing Prediction Fairness of AlphaFold2 in Drug Discovery – **Usman Abbas**, *Xingjian Shan, Jin Chen, Qing Shao*  Poster 27aa: Directed Evolution of an Alpha-Synuclein Degrading Enzyme — *Lawton Long*, *Cassidy Simas, Carl Denard* 

Poster 27ac: Meta-Analysis of Proteolytic Cleavage Specificity Using Machine Learning — **Suhyeon Kim**, Hyeju Song, Sumaiya Islam, Christopher Kieslich

Poster 27ad: 8-Oxo-7,8-Dihydroguanosine Alters RNA Degradation Behavior of Polynucleotide Phosphorylase – Lucas Miller, Shawn Schowe, Runhua Han, Vashita Jain, Sean Engels, Juan Camilo Gonzalez Rivera, Marino Resendiz, Lydia Contreras

Poster 27ae: Environmental Dependence of Collateral Fitness Effects — *Erh-Yeh Tsou*, Jacob D. Mehlhoff, Jacob D. Mehlhoff, Marc Ostermeier

Poster 27af: Novel Lasso Peptides Produced By Actinobacteria from the Atacama Desert – Valeria Razmilic, Juan Asenjo, Irene Martinez

Poster 27ag: Discovery and Characterization of a Structurally Unique Heterocyclic Peptide Enterolysin S – *Chengyou Shi*, *Marko Nesic, David Sarlah, Huimin Zhao* 

Poster 27ah: In Situ Characterization of Ammonia-Dependent Enzymes — Adam Caparco, Bettina Bommarius, Laurine Ducrot, Carine Vergne-Vaxelaire, Julie Champion, Andreas Bommarius

Poster 27aj: Artificial Lipid Biomembranes for Full-Length Sars-Cov-2 Receptor — *Ting Wang* 

Poster 27ak: Multiplexing of Cas Orthologs for Disease Detection — Briana Pizzano, Lilia Yang, Piyush Jain

Poster 27al: Programmable RNA Detection with CRISPR-Cas12a – Grace Shoemaker, Santosh R. Rananaware, Emma K. Vesco, Swapnil Anekar, Luke Samuel W. Sandoval, Katelyn Meister, Nicolas C. Macaluso, Long Nguyen, Piyush Jain Poster 27cl: Balancing Monoatomic Ion-Biomolecular Interactions in the Polarizable Drude Force Field — **Yiling Nan**, *Alexander D. MacKerell* 

# BIOSENSORS AND BIODIAGNOSTICS

Poster 27am: An Ultrasensitive Amplification-Free Nucleic Acid Detection Using CRISPR Chain Reaction v2 — *Minji Chang*, Santosh Rananaware, Carlos Orosco, Lilia Yang, Emma K. Vesco, Grace Shoemaker, Piyush Jain

Poster 27an: Nanopore Sequencing of 8-Letter Xenonucleic Acids — *Hinako Kawabe*, *Jorge A. Marchand* 

Poster 27ao: Dielectric Characterization of Babesia *Bovis* Using the Crossover Frequency Technique on a Point and Planar Electrodes Microfluidic Device – Raphael Oladokun, Soumya K. Srivastava

Poster 27aq: Quantifying Plasma Exosomes for Early Cancer Detection Using Rotational Brownian Motion of Janus Particles — John Sinclair, Sonu Kumar, Tiger Shi, Satyajyoti Senapati, Han-Sheng Chuang, Hsueh-Chia Chang

Poster 27ar: A Low-Cost Flow Cytometer for Blood Cell Analysis. — Mahrukh Mir

Poster 27as: Development of a Supercontinuum Laser-Based Confocal Microscope System for Excitation-Scanning Hyperspectral Imaging — *Silas J. Leavesley*, *Joel F. Andrews, Craig M. Browning, Megan Patterson, Mark S. Taylor, Thomas C. Rich* 

Poster 27at: A Rapid, Fully Automated Modular Electrochemical Platform Based on a Porous Flow-through Electrode for Sensing Biological Molecules of Interest — **Sagnik Basuray**, Yu-Hsuan Cheng, Zhenglong Li, Sreerag Kaaliveetil, Niranjan Haridas

Poster 27au: A Point-of-Care Device Capable of High-Throughput Diagnostic Testing Using Recombinase Polymerase Amplification (RPA) – *Aubrey Schultz, Robert Beitle*  Poster 27av: PAM-Independent Detection of Nucleic Acid Targets with CRISPR-Cas12a – Santosh Rananaware, Katelyn Meister, Grace Shoemaker, Emma K. Vesco, Luke Samuel W. Sandoval, Jordan Lewis, Briana Pizzano, Piyush Jain

Poster 27aw: Production and Application of SARS-CoV-2 Pseudotyped Virus for Screening Antiviral Efficacy of Test Compounds on a High-Throughput Platform — *Maisha Feroz*, Seok-Joon Kwon, Yuefan Song, Jonathan Dordick

Poster 27ax: Nonfluorescent Ratiometric Sensing Utilizing CRISPR-Cas12a-Induced DNA Supercoil Relaxation – *Noor Mohammad*, *Logan Talton, Selen Dalgan, Qingshan Wei* 

# METABOLIC ENGINEERING

Poster 27ay: Engineering Corynebacterium Glutamicum for Biomanufacturing of β-Ketoadipate from Lignin-Derived Aromatics – Arren Liu, Tyler Okane, Nandini Kannoju, David Nielsen, Arul Mozhy Varman

Poster 27az: Engineering Novel Microbes for Upcycling Waste Plastic and Solving Climate Crisis — Yuxin Tian, Jinjin Diao, Yifeng Hu, **Tae Seok Moon** 

Poster 27ba: Continuous Production of Acetic Acid By *Eubacterium Limosum* KIST612 Using an External Membrane Module — *Myounghoon Moon, Gwonwoo Park, Min-Sik Kim* 

Poster 27bb: Enzymatic Optimization of the Biosynthetic Production of Paraxanthine By Site-Saturated Mutagenesis with Enhanced Formaldehyde-Sensitive Selection — *Meredith Mock*, *Margaret Kapperman, Camden Hutchison, Joseph Rodriguez, Kayla Pakulski, Nick Gleason, Ryan Summers* 

Poster 27bd: Harnessing Robustness of Thermophilic Bacillus Coagulans for Conversion of Switchgrass Hydrolysates to Designer Bioesters at Elevated Temperatures – David Dooley, Seunghyun Ryu, Jackson Edwards, Khanh Ha, Richard Giannone, Bruce S. Dien, Cong Trinh Poster 27be: Agent-Based Metabolic Modeling for the Rational Engineering of *Chlamydomonas Reinhardtii* — Sandra Gomez Romero, Nanette Boyle

# SYNTHETIC BIOLOGY AND APPLICATIONS

Poster 27bf: Engineering High-Throughput Fluorescent Reporters for Selenocysteine Incorporation — Devon Kulhanek, Qiyao Wei, Zach Jansen, Andrew Gilmour, Ross Thyer

Poster 27bg: Feedforward Loop-Based Antithetic Controller for Improved Adaptation Dynamics — *Thales Spartalis, Xun Tang* 

Poster 27bh: Single and Multiplexed Gene Repression in Solventogenic *Clostridium* Via Cas12a-Based CRISPR Interference – *Rochelle Joseph*, *Nicholas Sandoval* 

Poster 27bi: Streamlined Yeast Cell Reactors with Residence Time Control to Engineer and Profile Protein-Modifying Enzymes — Sage Nelson, Samantha Martinusen, Lawton Long, Ethan Slaton, Carl Denard

Poster 27bj: Heterologous Derived Proteins Tethered to the Surface of Yeast: Arming Saccharomyces Cerevisiae with Sars-Cov-2 Receptor Binding Domain and Green Fluorescent Protein. — Shadrach Ibinola, Hazim Aljewari, Sebastian Freeman, Vicki Thompson, Kaiming Ye, Robert Beitle

Poster 27bk: Investigating the Relaxase Behavior and Replication Functionality of the Mobilization Protein *Mobv* in the Plasmid pBBR1 — *Mark Kathol*, *Cheryl Immethun*, *Dianna Morris*, *Rajib Saha* 

Poster 27bl: Leveraging the Carbon Storage Regulatory Network to engineer Complex Post-Transcriptional Gene Circuits — Trevor Simmons, Gina Partipilo, Anna Stankes, Darian Chiu, Benjamin Keitz, Lydia Contreras Poster 27bm: Dynamic DNA Nanoaggregation Driven By Ionic Self-Association — **Sneha Mukherjee**, Kevin Lin, Albert J. Keung, Orlin D. Velev

Poster 27bn: Engineering of Tunable Cell Network with Endogenous Template Activation of Non-Excitable Cells – Junkai Xie, Bo-Chuan Huang, Chongli Yuan

Poster 27bo: Assemblytron: Flexible Automation of DNA Assembly with Opentrons OT-2 Lab Robots – John Bryant Jr., Mason Kellinger, Cameron Longmire, Ryan Miller, Clay Wright

Poster 27bp: Bringing Physical Signals into Cell-Free Expression – Junzhu Yang

Poster 27bq: Engineered Biological Security Systems: Introducing Biotic Cryptography and Encryption – **Dowan Kim**, Ishita Kumar, Corey Wilson

Poster 27br: Specific Codons Control Cellular Resources and Fitness — *Nikhil U. Nair* 

Poster 27bs: Glutathione-Responsive Disulfide-Containing Poly (β-amino esters) Nanogels for Drug Delivery Applications — Anastasiia Aronova, Alea Smith, Brittany Givens Rassoolkhani, Thomas D. Dziubla

# SYSTEMS AND QUANTITATIVE BIOLOGY

Poster 27bt: Regulating Cell Function to Accelerate Bone Cell Growth Using Micro- to-Nano Crumpled Mxene Multilayers. — Mohammad Asadi Tokmedash, Jouha Min

Poster 27bu: Framework for Optimizing Modulations of Enzyme Expression Levels and Kinetic Parameters for Computational Microbial Strain Design – *Patrick Suthers, Mengqi Hu, Costas D. Maranas* 

Poster 27bv: Investigating the Effects of Surface Stiffness on Human Mesenchymal Stem Cell Immunomodulatory Potential – Sara Olsen, Bethany Almeida Poster 27bw: Caffeine Affects Horizontal Gene Transfer in Bacteria — **Tracy Mei**, Robert Jinkerson, Qing Sun

Poster 27bx: Illuminating Cell Entry Pathways of Sars-Cov-2 By Replicating Distinct Host Environments on a Bioelectronic Sensor – Susan Daniel, Zhongmou Chao, Ekaterina Selivanovitch, Konstantinos Kallitsis, Zixuan Lu, Alberto Salleo, Roisin Owens

Poster 27by: Deep Neural Networks for Predicting Single Cell Responses and Probability Landscapes — *Heidi E. Klumpe*, *Jean-Baptiste Lugagne, Ahmad S. Khalil, Mary J. Dunlop* 

Poster 27bz: The Effects of Pfas-Induced Activation of ER Stress Sensor IRE10 and Its Downstream Pathways for DNA Damage Repair – *Kevin Chen*, Sean Foster, Caleb Sandum, Sardar Murtaza, Elaina Gouin, S. Patrick Walton, Christina Chan

Poster 27ca: Investigation of Interaction of Stress Response, Virulence, and Antibiotic Resistance in *Listeria Monocytogenes* through Protein Network Analysis – *Robert Hanes Jr., Zuyi Huang, Fangyuan Zhang* 

Poster 27cb: Development of a Genome-Scale Metabolic Model for Auxenochlorella Protothecoides to Enable Rational Engineering – Mark Vigliotti, Jacob Tamburro, Nanette Boyle

Poster 27cc: Bacterial Metabolites Required for Post-Embryonic Development in *C. Elegans — Min Feng, Luis R. Garcia, Qing Sun* 

Poster 27cd: Analysis of Pmad and Medea Expression in BMP Pathway in S2 Cells and Drosophila Germline Stem Cells Niche – Hung-Yuan Chen, Gregory Reeves

Poster 27ce: Expression of Glycolytic Genes in NAFLD Correlates with the Risk of Hepatocytes Dysfunction - Samantha Harvat, Srivatsan Kidambi Poster 27cf: A Systems Engineering Computer-Assisted Biomarker Detection Framework for Autism Spectrum Disorder Using Proteomic Data — Farnaz Yousefi Zowj, Q. Peter He

Poster 27cg: An SPNS1-Dependent Lysosomal Lipid Transport Pathway That Enables Cell Survival Under Choline Limitation — Wentao Dong, Samantha Scharenberg, Ali Ghoochani, Kwamina Nyame, Roni Levin-Konigsberg, Aswini Krishnan, Eshaan Rawat, Kaitlyn Spees, Michael Bassik, Monther Abu-Remaileh

Poster 27ch: A Novel Method to Measure Transcriptional Maturity of Engineered Liver Cells – Daniel Guiggey, Natesh Parashurama

Poster 27ci: Multi-Omic Characterization of CHO Cells Reveals Fluxomic Diversity and Amino Acid Utilization Bottlenecks in High-producer Clones

– Saratram Gopalakrishnan,
William Johnson, Miguel Angel
Valderrama-Gomez, Elcin Icten,
Cleo Kontoravdi, Nathan Lewis

Poster 27cj: Constraining the Predictions of Conserved SMAD Signaling Pathway through Parameter Identifiability Informed Experimental Design. – *Razeen Shaikh, Gregory Reeves* 

Poster 27ck: Using Experimentally Validated ML Models to Predict the Thawing Time of Biologics during Large Scale Freeze-Thawing Cycles — Venkatraman Nagarajan, Bodhisattwa Chaudhuri, Bruna Minatovicz, Lauren Fontana, Tibo Duran, Tanu Mehta, Yangchao Luo, Yi Wang

(28) Poster session: Engineering Fundamentals in Life Science

Monday, Nov 6, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

Shreyas Rao, Chair

**Sponsored by:** Engineering Fundamentals in Life Science

**Poster 28b:** Engineering an α-P-Selectin Antibody for Quantifying Drug Delivery in Glioblastoma – **Omar Abed**, Timon Lwo, Colin Greineder, James Moon Poster 28c: Novel Treatment of Streptococcus Pneumoniae and Nontypeable Haemophilus Influenzae-Coinfected Otitis Media – Xiaojing Ma, Rong Yang

Poster 28d: Combining Targeted α-Particle Therapy with Chemotherapy: A Two-Pronged Approach to Combat Breast Cancer Brain Metastases — *Pooja Hariharan, Stavroula Sofou* 

Poster 28e: Experimental and Simulation Investigation on Application of Metal-Organic Frameworks to Multi-Drugs Carrier – Ayumi Ohashi, Kazuki Ohshima, Shuji Ohsaki, Hideya Nakamura, Satoru Watano

Poster 28f: Optogenetic-Mediated Preconditioning As a Novel Approach to Protect Cells from Stress-Induced Injury – **Seulhee Kim**, Patrick Ernst, Xiaoguang Liu, Lufang Zhou

Poster 28g: A Matlab-Based Analysis of the Dynamics and Organization of *Staphylococcus Aureus* Surface Adhesion in a Bioflux 200 System – **Sarees Shaikh**, Patrick Ymele-leki

Poster 28h: Survival of Aging CD264<sup>+</sup> and CD264<sup>-</sup> Populations of Human Bone Marrow Mesenchymal Stem Cells Is Independent of Colony-Forming Efficiency – Sean Madsen, Alan Tucker, Margaret Giler, Katie Russell, Georgina Dobek, Mimi Sammarco, Bruce Bunnell, **Kim** O'Connor

Poster 28: Versatile, Rapid, and Trackable Light-Activated Drug Release from Nanocarriers Using a Photo-Cleavable Prodrug Approach for Precise Immuno-Oncology. — Amy Moreno, Jennifer Vilnot, Victoria Hempstead, Stefan Chassaing, Nathalie Pinkerton

Poster 28j: Apoptotic Effects of Low Molecular Weight Fucoidan Released from PEGDA Nano-Particles Encapsulated in Chitosan on MDA-MB-231 and MCF-7 Cell Lines – *Hazim Aljewari, Raquel de Castro, Robert Beitle, Audie Thompson*  Poster 28k: Microfluidic Oscillators Enable Dynamic Concentration Flow Profiles – Xiaoqian Wang, Priyan D. Weerappuli, Sasha Cai Lesher-Pérez

Poster 28I: Leveraging Synergy of Hitchhiking Nanocarriers and Chemotherapy to Overcome Delivery Challenges in Glioblastoma – *Aira Sarkar*, *Rangaramanujam Kannan*, *Stavroula Sofou* 

Poster 28m: Customized Biodegradable 3D-Printed Bone Grafts with Biomimetic Porosity - Nilesh R Bhoi, Jayesh Bellare

Poster 28n: Engineering a 3D Multilayer Multicellular Model of Endometrial Cancer for High Throughput Drug Screening with paclitaxel Loaded Poly (caprolactone) Nanoparticles — Ines Cadena Cabezas, Claire Rowlands, Brittany Givens Rassoolkhani, Kaitlin Fogg

Poster 280: Optimization of Functionalized Hydrogels for iPSC-Derived Midbrain Dopaminergic Neuron Culture – *Nicole Marguerite, Ethan Lippmann* 

Poster 28p: Aged and Young Breast Matrix Bound Vesicles in Breast Cancer – Jun Yang, Gokhan Bahcecioglu, George Ronan Jr., Pinar Zorlutuna

Poster 28q: 3D-Printed Implantable Neural Arrays Based on Templated Conductive Polymer Electrodes – **Seoyeon Won**, *Huanan Zhang* 

Poster 28r: The Sars-Cov-2 Virus at Interfaces: A Molecular Dynamics Simulation Study — *Florian Fleckenstein, Hans Hasse, Simon Stephan* 

Poster 28s: Multivalent Anchoring of Cell Wall Binding Domains By Using Split Fluorescent Proteins — *Shirley Xu*, Inseon Lee, Seok-Joon Kwon, Jonathan Dordick

Poster 28t: Promising Routes for Mitigating RBC Storage Lesions in As-3 — Linh Tran, Cristina González-Fernández, Stefano Ciannella, Mitchell Weigand, Jacob Strayer, Xian Wu, Hyeon Choe, Eugenio Bringas, Inmaculada Ortiz, Jeffrey Chalmers, Jenifer Gomez Pastora Poster 28u: Evaluation of Structure-Activity Function of a Lasso Peptide Using High-Throughput Screening — *Alina Thokkadam, Truc Do, A. James Link* 

Poster 28v: Designing Recombinant Protein-Based Sensory Vesicle System — Bornita Deb, Adriana LaVopa, Jackson Powers, Carl Denard, Yeongseon Jang

Poster 28w: Artificial Intelligence-Based Parametrization of Next Generation Systems Biology Models – Achilleas Karakoltzidis, Spyros Karakitsios, Dimosthenis Sarigiannis

Poster 28x: Miner: An Ontology-Based Approach for Advancing Toxicological and Public Health Sciences – Achilleas Karakoltzidis, Spyros Karakitsios, Dimosthenis Sarigiannis

Poster 28y: Enhancing Next Generation Systems Biology Models with Deep Learning for Initial Conditions Specification – Achilleas Karakoltzidis, Spyros Karakitsios, Dimosthenis Sarigiannis

Poster 28z: Modeling Nanocarrier Efficacy in a Three-Dimensional Multicellular Model of Endometrial Cancer — *Claire Rowlands*, *Brittany Givens Rassoolkhani, Ines Cadena Cabezas, Kaitlin Fogg* 

Poster 28aa: M2 but Not M1 Macrophages Can be Induced to Migrate Against the Direction of Shear Flow — Aman Mittal, Alexander Buffone Jr.

Poster 28ab: The Potential of Tetrahydrobiopterin As an Early Biomarker of Cardiovascular Diseases: A Computational Analysis – Saptarshi Kar, Hala Al Amrani, Shahad Almutairi

Poster 28ac: Aspa Mediated Persistence State in Escherichia coli – **Rauf Shiraliyev**, Sayed Golam Mohiuddin, Mehmet Orman

Poster 28ad: Development of a Genetically-Encoded Delivery Vehicle for Biomoleculedelivery into Plants – *Mark Legendre*, *Gözde Demirer*  Poster 28ae: Application of Metal-Organic Frameworks for Pharmaceutics Fields: Improvement of Water Solubility and Multi-Drugs Carrier — **Shuji Ohsaki**, Ayumi Ohashi, Kazuki Ohshima, Hideya Nakamura, Satoru Watano

Poster 28af: On-Demand Electrochemically Controlled Fluorescein Release from an Ultrasonically Powered Implant – Mohammad Mofidfar, Max L. Wang, Christian F. Chamberlayne, Haixia Xu, Spyridon Baltsavias, Justin P. Annes, Amin Arbabian, Richard Zare

Poster 28ag: Investigating Synthetic Biological Membranes with Sensitivity to Low-Strength Electric Fields — *Thomas Kinard, Steven P. Wrenn* 

Poster 28ah: Role of Extracellular Vesicles in Maintaining Stemness in Breast Cancer Metastasis

– Spenser Brown, Yifei Sun,
Joseph Danner, Steven Weinman,
Yonghyun (John) Kim

Poster 28ai: A Microphysiological System for Modeling Enteric Neuron and Epithelium Interactions in the Gut – *Kyla Nichols, Abigail Koppes, Ryan Koppes* 

Poster 28aj: A Microbead-Based Artificial Germinal Center (aGC) Model for the Proliferation and Differentiation of Human B Cells in Vitro — *Pearlson Prashanth Austin Suthanthiraraj, Kyung-Ho Roh* 

Poster 28ak: Investigating the Role of H<sub>2</sub>s in Liver Fibrosis - Neeti Gandhi, Kaleb Chan, Emma Henderson, Ishani Sarkar, John Matson, Padmavathy Rajagopalan

(29) Poster session: Food and Bioprocess Engineering

Monday, Nov 6, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

Sitanan Thitiprasert, Chair Maobing Tu, Co-Chair

Sponsored by: Food

Poster 29a: Influence of Citric Acid Pretreatment and Different Temperatures on the Convective Drying of Banana – *Adriano Souza*, *Manuela Duarte*, João H. *Fernandes da Silva*, *Shirley C*. *Rupert Brandão*, José Moura, *Rafael A. Batista de Medeiros*, *Patricia Azoubel* 

Poster 29b: Preparation of Low-Sugar Jujube Powder through Facultative Anaerobic Fermentation Process As Prebiotcics – *Tianhao Chen, Huiren Zhuang, Zhenghuan Yang, Yalin Zhou, Guogiang Jiang* 

Poster 29c: Production of Rice Bran Oil from Rice Bran By Using Solvent Extraction Technique - Syed Farzan Ali Shah

Poster 29e: Fungally and Bacterially Antifouling Coatings for Galvanized Steel Surfaces — Shuhao Liu, Wentao Zhou, Minchen Mu, William DeFlorio, Sang Ha Song, Ha Young Choi, Luis Cisneros-Zevallos, Jun Kyun Oh, Mustafa Akbulut

Poster 29f: Optimisation of Microbial Protein Fermentation, Using a Hybrid of Learning-Based Control and Model Predictive Control. – *Tom Vinestock, Miao Guo* 

Poster 299: Integrated Fermentation Process with Microbial Consortia for Acetate Production from Lignocellulosic Biomass – *Surya Tamang*, *Momodou Sowe, Jie Dong* 

Poster 29h: Improving Efficacy of Cyclophosphamide in the Treatment of Murine Colon Cancer By Remodulating Gut Microbiota with Jujube Powder – *Huiren Zhuang, Nan Jing, Luoyang Wang, Guoqiang Jiang, Zheng Liu* 

Poster 29i: Recent Advances in the Employment of Probiotics for the Syntheses of Bacteriocins, Sugar Alcohols, Bioactive Peptides and Other Food Additives — Bababode Kehinde,

Oluwakemi Igiehon, Ishrat Majid

Poster 29k: Oyster Mushroom Drying in Tray Dryer: Parameter Optimization, Drying Kinetics and Characterization — **Talbachew Tadesse Nadew**, Ali Shemsedin Reshad, Petros Demissie Tegenaw Poster 29I: Uncovering the Role of Impurity Sugars on the Crystallization of D-Tagatose Crystal: Experiments and Molecular Dynamics — **Dongbo Wang**, Dandan Han, Junbo Gong

Poster 29m: De Novo Biosynthesis of Butyl Butyrate Using Heterologous Lipase in *Clostridium Tyrobutyricum* – Geng Wang, Shang-Tian Yang

Poster 29n: Carbon-Economic Biosynthesis of Polymalic Acid and Malic Acid from Ethanol and Biomass Feedstocks – *Xiang Zou* 

Poster 290: Enhanced Butanol Production from Lignocellulose Hydrolysate By Engineered *Clostridium Tyrobutyricum* with Alleviated Glucose-Mediated Carbon Catabolite Repression – **Qingke Wang**, Shang-Tian Yang

Poster 29p: A Cotransformation Strategy for Combinatorial Engineering Paralogous Genes in *Clostridium Acetobutylicum* – Chao Zhu, Zixuan Wang, Chuang Xue

Poster 29q: Biochar Regulates Anaerobic Metabolism for Increased Production of Biohydrogen — *Weiming Li, Chi Cheng, Meng Liu, Shang-Tian Yang, Nangi Ren* 

Poster 29r: Disrupting Sporulation in Engineered *C. Tyrobutyricum* Strain Showed Increased Butanol Production and More Stable Bioprocess – *Zonghao Zhang*, *Shang-Tian Yang* 

Poster 29s: Energy-Efficient Butanol Production By Clostridium Acetobutylicum with Histidine Kinase Regulation to Improve Strain Tolerance and Process Robustness — *Chuang Xue, Chao Zhu, Youduo Wu* 

Poster 29t: Metabolic Engineering of *Clostridium Tyrobutyricum* for Butyl Butyrate Production from Glucose and Mannitol – *Jufang Wang* 

Poster 29u: Fixing Carbon Dioxide in Situ during Ethanol Production By Formate Dehydrogenase - Wenjie Yuan, Cong Du, Yimin Li Poster 29v: Metabolic Engineering of *Thermoanaerobacterium Aotearoense* SCUT27 for Biofuels Production from Sucrose and Molasses — *Hongxin Fu* 

Poster 29w: Engineering Self-Assembled Nanoreactors for Enhanced Biocatalysis – We Kang

Poster 29x: Transforming How the World Makes Chemicals:Sustainably Produced Bio-Based Chemicals that are Made to Scale <sup>TM</sup> − Jacob Wolf, Trevor Rosensohn, Zhixia Ye

# (30) Poster Session: Nanoscale Science and Engineering Forum

Monday, Nov 6, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

Yoonjee Park, Chair Avery Zheng, Co-Chair

**Sponsored by:** Nanoscale Science and Engineering Forum

Poster 30a: Electrochemical Windows of Sulfone-Based Electrolytes for Lithium Metal Batteries: A Density Functional Theory and Cluster-Continuum Model Investigation — *Minhee Park*, *JunBeom Cho, Bumjoon Seo, Won Bo Lee* 

Poster 30b: Uniformly Embedded Cobalt Phosphide Nanoparticles in Carbon Nanofibers As Sulfur Host Via Co-PBA in-Situ Growth for High-Performance Li-S Batteries – *Zhi Liu*, *Cameron Romero*, *Kenneth Gordon*, *Le'Naedrea Moore*, *Ling Fei* 

Poster 30c: Modeling Elastic Properties of Hydrogel Depending on Effective Structures Using Mixed Force-Field Coarse Graining Method — Seunghyok Rho

Poster 30d: High Resolution Measurement of Potential-Dependent Electrochemical Activities on HOPG Using Scanning Electrochemical Cell Microscopy (SECCM) - Myunghoon Choi, Sang-Joon Cho, Lane Baker, Stefan Kaemmer

Poster 30e: Wetting Transparency of Free-Suspended Single-Layer Graphene on Liquid Substrate. — Fan Yang, Annette Thompson, Lei Li Poster 30f: Feedback Control System of Iron Catalyst in Reactors Using Deep-Injection Floating Catalyst Chemical Vapor Deposition (DI-FCCVD) – *Mingrui Gong, AnaVi Benavides Figueroa, Arthur Sloan, Matteo Pasquali* 

Poster 30g: Facile Synthesis of Halogen Terminated Mxene from Different MAX Phases for Electromagnetic Interface Shielding — *Shane Reed*, *Pitchaimari Gnanasekar, Sanjay Singh, Natalie Arnett, Dinadayalane Tandabany, Theo Siegrist, Subramanian Ramakrishnan* 

Poster 30h: Rheo-Electric Investigation of Carbon Black Suspensions Undergoing Shear-Induced Microstructural Rearrangement — *Paolo Ramos*, *Julie Hipp, Jeffrey Richards* 

Poster 30i: Lyotropic Liquid Crystals of Cellulose Nanocrystal/Boron Nitride Nanotube Mixtures: Phase Behavior and Aligned Assemblies – Eren Katnas, Geyou Ao

Poster 30j: Scalable Manufacturing of Inorganic Nanomaterials Using Jet Mixing Reactors – **Priya Jana**, Faiz Khan, Pinaki Ranadive, Jessica Winter, Nicholas Brunelli

Poster 30k: Threshold and Excess Electrolyte-to-Sulfur (E/S) Ratios in Lean-Electrolyte Li-S Batteries - Xiaosi Gao, Siddharth Tiwari, Aditya Pandey, Yiqi Shao, Ziang Gao, Yong Lak Joo

Poster 301: Glycopolymer-Wrapped Carbon Nanotubes Detection of Viral Proteins - Brandon Heppe, Geyou Ao,

Xue-Long Sun

Poster 30n: Polymer-Cerium Oxide Nanocomposites Synthesized By Hydrothermal Method for Bone Tissue Regeneration Applications – Shreya Pawar

**Poster 30o:** Surface Modifications to Functionalized Outer Coating of Magnetic Nanoparticles to Target Medical Dyes in Solution and Their Impact on Contaminated Water Compositions. — *Evan Wetmore*, *Keisha Walters*  Poster 30p: Creation of Carbohydrate-Decorated Organic Color Centers Via Copper-Free Click Chemistry — *Nina Dzombic*, *Joseph Keil, Xue-Long Sun, Geyou Ao* 

Poster 30q: Lipid Nanoparticle Structure and Immune Response Regulate mRNA Organ Tropism and Pup Growth during Pregnancy in Mice. – Namit Chaudhary, Alexandra Newby, Mariah Arral, Saigopalakrishna Yerneni, Samuel LoPresti, Rose Doerfler, Daria Petersen, Bethany Fox, Tiffany Coon, Angela Malaney, Yoel Sadovsky, Kathryn Whitehead

Poster 30r: The Particle Drifting Effect – Impact of Membrane, Sink Condition, Particle Size, Drug Solubility, and Colloid Type – *Na Li* 

Poster 30s: h<sup>6</sup> Organometallic Hexagonal Boron Nitride: Functionalization and Prope – *Kartikey Sharma* 

#### (31) Poster Session: Decarbonization by Electrification

Monday, Nov 6, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

Elizabeth Biddinger, Chair Miguel Modestino, Co-Chair Ignasi Palou-Rivera, Co-Chair Dharik Mallapragada, Co-Chair

**Sponsored by:** Decarbonization of the Chemical Industry through Electrification

Poster 31a: Modeling and Techno-Economic Assessment of an Airto-Syngas Process — *Hussain Almajed*, Omar J. Guerra, Wilson A. Smith, Bri-Mathias Hodge, Ana Somoza Tornos

(32) Issues in Law for Practicing Engineers

Monday, Nov 6, 3:30 PM Hyatt Regency Orlando, Bayhill 26

**Sponsored by:** Chemical Engineering & the Law Forum

**4:00 Paper 32a:** How to Protect Your Intellectual Property in the Academic World – *Paul Townsend*, *Charles Collins-Chase*, *Lauren Dowty*  **4:30** Paper 32b: Obviously New or Just a Copy – Engineers Play a Critical Role in Evaluating Patent or Trade Secret Infringement Claims – Achim Wechsung, David Hietala

(33) Invited Session In Honor of Prof. Babatunde A. Ogunnaike

Monday, Nov 6, 3:30 PM Hyatt Regency Orlando, Bayhill 25

Ali Mesbah, Chair Masoud Soroush, Co-Chair

**Sponsored by:** Systems and Process Control

**3:30 Paper 33a:** A Career of Excellence and Service — *Levi Thompson* 

**3:55 Paper 33b:** Tunde's Contributions to Advanced Process Control – *Lorenz Biegler* 

4:20 Paper 33c: On Using Feedback Control to Contend with Nature's Randomness – James Rawlings, Robert McAllister

**4:45 Paper 33d:** Distributed Statistics – Some Challenges – *Christos Georgakis* 

**5:10 Paper 33e:** Modeling and Control of Biopharmaceutical Manufacturing – *Richard Braatz* 

5:35 Paper 33f: Connecting Engineering and Biomedicine in Closed Loop to Study Heart and Liver Diseases — *Rajanikanth Vadigepalli* 

(34) Process Intensification and Modular Manufacturing: Intensified Reaction and Separation Processes

Wednesday, Nov 8, 3:30 PM Hyatt Regency Orlando, Celebration 16

Patricia Gillenwater, Chair Julia Faeth, Co-Chair

Sponsored by: Process Intensification & Modular Chemical Processing 3:30 Paper 34a: Modular Manufacturing of Active Pharmaceutical Ingredients (APIs): Novel Approaches for Continuous Heavy Metal Removal from API Syntheses Solutions – Daniel Moser, Joscha Boehm, Peter Neugebauer, Heidrun Gruber-Woelfler

**3:50 Paper 34c:** Process Intensification of Electrodialysis through the Investigation and Elimination of Maldistribution — Jack Ledingham, **Alasdair Campbell**, Jonathan R Howse, Elliot Tyndale-Biscoe, Kyra Sedransk Campbell

4:10 Paper 34d: Intensification of Polymer Production Using Ultrasound: The Polyurethane Case As Example – *Ariana Bampouli*, Sofie Scheers, Quinten Goris, Joachim Demaerel, Wim De Borggraeve, Georgios D. Stefanidis, Tom Van Gerven

**4:30 Paper 34e:** Process Design and Intensification of a Continuous Modular Crystallization System — *Monika Neal, Montgomery Smith, Zoltan Nagy* 

**4:50** Paper 34f: Research and Development on Purification Technology of High-Purity Hexane and High-Purity Benzene - *Zhongfeng Geng*, Hao Gong, Yingzhe Yu, Haoxi Jiang, Minhua Zhang

(35) Invited: Celebrating 30 years of the PTF (Last 15 years)

Monday, Nov 6, 3:30 PM Hyatt Regency Orlando, Bayhill 21

Liang-Shih Fan, Chair James Gilchrist, Co-Chair

Sponsored by: Particle Technology Forum

**3:30** Paper 35a: Advances in the Simulation of Dry Powder Inhalation Flows — *Sankaran Sundaresan* 

**3:48 Paper 35b:** People and Tools Advancing the Science of Particle Technology — *Richard Lueptow* 

**4:06 Paper 35c:** Ten years at PTF: Connect fundamental research with industrial scale problem solving — *Yi Fan*  **4:24 Paper 35e:** Progress in wet granulation process development from a pharmaceutical industry application perspective - *Maitraye Sen* 

**4:42 Paper 35f:** Spherical Agglomeration as a Tool for Manufacturing of Formulated Products: Mechanistic Understanding and Mathematical Modelling — *Rachel Smith* 

5:36 Paper 35d: Particle Technology and Clean Energy Transition for Sustainable Future — *Ah-Hyung Alissa Park* 

(36) Feedstock Conversion Interface Consortium – Understanding Feedstock Variability to Enable Next Generation Biorefineries (Invited Talks)

Monday, Nov 6, 3:30 PM Hyatt Regency Orlando, Regency Ballroom T

Jordan Klinger, Chair Edward Wolfrum, Co-Chair Vicki Thompson, Co-Chair

**Sponsored by:** Sustainable Biorefineries

**3:30** Paper 36a: Biological Degradation and Moisture Effects on Corn Stover Comminution — *Tiasha Bhattacharjee, Jordan Klinger, Noah Berglund, Bradley Wahlen, Vicki Thompson, Yidong Xia, Neal Yancey* 

**3:49 Paper 36b:** Impacts of Municipal Solid Waste Feedstock Variability on Bench-Scale Gasification – *Dan Dupuis* 

**4:08 Paper 36c:** Experiment-Informed Virtual Physics for Granular Feedstock Preprocessing and Handling Operations: Overview of Recent Progress — **Yidong Xia**, Wencheng Jin, Ahmed Hamed, Jordan Klinger, Nepu Saha, Tiasha Bhattacharjee, Mark Small, Neal Yancey, C. Luke Williams, John E. Aston, David Thompson, Lynn Wendt, Vicki Thompson

4:27 Paper 36d: Assessment of the Abrasiveness of Biomass and MSW Feedstock Particulate Materials – **Oyelayo Ajayi**, George Fenske, Jun Qu, James Keiser, Jeffrey A. Lacey, Vicki Thompson, Miranda Kuns 5:05 Paper 36f: Failure Modes and Effects Analysis of Biorefinery Pathways — **Rachel Emerson**, Pralhad Burli, Lorenzo Vega-Montoto, Tiasha Bhattacharjee

#### (37) Area Plenary: Carbon Nanomaterials (Invited Talks)

Tuesday, Nov 7, 8:00 AM Hyatt Regency Orlando, Discovery 43

Geyou Ao, Co-Chair Anju Gupta, Co-Chair

**Sponsored by:** Carbon Nanomaterials

8:00 Paper 37a: Exploring the Best CVD Conditions for Growth of Small-Diameter Single-Wall Carbon Nanotubes Using an Autonomous Research System — Brian M. Everhart, Rahul Rao, Tsung Wei Liu, Diego Gomez Gualdron, Benji Maruyama, Placidus Amama

8:30 Paper 37b: Molecular Design and Investigation of 2-D Hybrid Materials – Sanket Deshmukh

#### (38) Area Plenary: Interfacial Phenomena (Invited Talks)

Tuesday, Nov 7, 8:00 AM Hyatt Regency Orlando, Orlando Ballroom N

Marina Tsianou, Chair Christopher Wirth, Co-Chair

**Sponsored by:** Interfacial Phenomena

(39) Tutorial Session on Electrochemical Methods, Systems and Applications (Invited Talks)

Tuesday, Nov 7, 8:00 AM Hyatt Regency Orlando, Orlando Ballroom M

Abdoulaye Djire, Chair Wesley Chang, Co-Chair Elizabeth Corson, Co-Chair Magda Barecka, Co-Chair

**Sponsored by:** Electrochemical Fundamentals

8:00 Paper 39a: Electrocatalysis for Carbon Dioxide Utilization — Feng Jiao

8:35 Paper 39b: Localized Statesof-Charge in Battery Electrodes: Using Microscopic X-Ray Diffraction Data to Solve Current Distributions – Joshua Gallaway

**9:10** Paper 39c: Designing Electrochemical Interfaces for Small Molecule Activation — *Sara Thoi* 

9:45 Paper 39d: An Introduction to Combining Electroanalysis with Microkinetic Modeling – *Maureen Tang* 

(40) Topical Plenary: Frontiers in Green Process and Product Engineering (Invited Talks)

Tuesday, Nov 7, 8:00 AM Hyatt Regency Orlando, Bayhill 18

**Sponsored by:** Green Process and Product Engineering

8:00 Paper 40a: Systems Analyses of Green Ammonia As a Sustainable Energy Carrier — *Qi Zhang* 

8:35 Paper 40b: Sustainable Aviation Fuel from Methanol and Ethanol Intermediates

Karthikeyan Ramasamy

**9:10** Paper 40c: Electrochemical Approaches to Decarbonizing Fuels and Chemicals – *Haotian Wang* 

(41) Charting Your Course from Academia to a Successful Professional Career (Panel Discussion/Workshop)

Tuesday, Nov 7, 8:00 AM Hyatt Regency Orlando, Regency Ballroom Q

Carmen Daoud, Chair Marissa Martine, Co-Chair

**Sponsored by:** Early Career Community (ECC) - Formerly YPC

# (42) Laboratory and Pilot Plant Safety

Tuesday, Nov 7, 8:00 AM Hyatt Regency Orlando, Bayhill 28

David Edwards, Chair Pratik Bhishikar, Co-Chair Tsatsral Battsengel, Co-Chair

Sponsored by: Pilot Plants

8:00 Paper 42a: Electrically Heated Equipment Safety in Pilot Plants — *Richard Palluzi* 

8:25 Paper 42d: What to Expect When Expecting in Lab: Safety Considerations and Green Chemistry Resources for Pregnant Researchers in the Chemical Laboratory — Mary Kate Lane, Paul T. Anastas, Julie B. Zimmerman

**8:50 Paper 42b:** Evaluation of Filler Containing Si-H (Silicon hydride) Formulations for H<sub>2</sub> off-Gassing Risks during Production and Packaging — *Hulusi Turgut*, Jeff Kelly, Nate Stelzer, Craig Gorin, Chi-Hao Chang, Rocky Zhu, Travis Scholtz, Ryan Gilliland, Michael Whitbrodt, Jyo Lyn Hor, Zach Rolfs

9:15 Paper 42c: Overlooked Considerations during Safety Reviews of Lab Scale Systems and Pilot Plants — *Pratik Bhishikar* 

9:40 Paper 42e: Utilizing Simple Heat Transfer Models for Safe Scale-Ups of Exothermic Chemistries – Jessica Nichols, Seshasayee Mahadevan, Jason S. Fisk, Mike DePierro, Jeff Kelly

**10:05 Paper 42f:** Utilizing a Digital Process Safety Game to Improve Training Strategies in Pilot Plants — **Brittany Butler**, Cayla Ritz, Jeffrey Stransky, Cheryl A. Bodnar, Emily Dringenberg, Elif Miskioglu

(43) Distillation and Absorption Processes Fundamentals, Developments, Optimization, and Applications I

Tuesday, Nov 7, 8:00 AM Hyatt Regency Orlando, Manatee Spring II

Gregory Cantley, Chair Izak Nieuwoudt, Co-Chair

**Sponsored by:** Distillation and Absorption

8:25 Paper 43a: Numerical Simulation of Fluid Dynamics and Mass Transfer of a Two-Phase Flow in Structured Packings — Marc Xia, Sebastian Rehfeldt, Harald Klein

8:50 Paper 43b: Will Laboratory and Pilot Plant Columns Soon be Superfluous? – *René Pöschmann*, Georg Brösigke, Markus Illner, Juergen Paschold, Steffen Mueller, Christoph Hiller, Laura-Selin Harding, Nico Lachmann, Ilja Ausner, Ansor Gaebler, Jens-Uwe Repke

9:15 Paper 43c: Azeotropic Refrigerant Mixture Separation Using Extractive Distillation with Ionic Liquids Entrainers — Abdulrhman Arishi, Mark B. Shiflett

**9:40 Paper 43d:** Dynamic Behavior of a Multiple Dividing Wall Column – a Theoretical and Experimental Study – **Yannick Waibel**, Lena-Marie Ränger, Thomas Grützner

10:05: Break

**10:30 Paper 43f:** Quantifying the Point Efficiency of a Distillation Column Under Non-Total Reflux Mode of Operation — *Rukhsar Ahmed*, *Tony Cai, Izak Nieuwoudt, Sayeed Mohammad, Clint Aichele* 

(44) Sustainable Engineering Forum Plenary Session (Invited Talks)

Tuesday, Nov 7, 8:00 AM Hyatt Regency Orlando, Regency Ballroom V

Ana I. Torres, Chair Magda Barecka, Co-Chair Ramalingam Subramaniam, Co-Chair

Sponsored by: Sustainable Energy

8:00 Paper 44b: Green Ammonia for Sustainable Energy and Agriculture — *Prodromos Daoutidis* 

8:45 Paper 44a: Machine Learning Boosted Catalyst and Operation Design for Clean Energy - Fanglin Che

**9:30 Paper 44c:** Establishing a Circular Economy in the Food Industry – *Mariano Martin* 

(45) Women in Engineering [WIC] Keynote & Breakfast -TICKETED EVENT - OPEN TO ALL

Tuesday, Nov 7, 9:00 AM Hyatt Regency Orlando, Windermere Ballroom X

## Ashley Bird, Chair

Sponsored by: Women in Chemical Engineering Community (WIC)

9:00 Paper 45a: Women in Engineering (WIC) Keynote — *Erin Kane, Ariel Furst* 

(46) Education Division Awards Plenary (Invited Talks)

Tuesday, Nov 7, 12:30 PM Hyatt Regency Orlando, Bayhill 30

Benjamin Davis, Chair Christy West, Co-Chair

Sponsored by: Education

**12:30 Paper 46a:** Navigating Professional Service When It's Personal — *Anthony Butterfield* 

**1:00 Paper 46b:** Cooperative, Hands-on, Active, Problem-Based Learning – Ideas & Insights for the Classroom – *Bernard Van Wie* 

**1:30 Paper 46c:** Engineering Illustrated: Engaging Students' Interest, Confidence, and Understanding through STEM Comics and Videos – *Luke Landherr* 

2:00 Paper 46d: Enhancing Research Impact through Meaningful and Strategic Service - Sindia M. Rivera-Jimenez

(47) Fundamental Research in Transport Processes

Tuesday, Nov 7, 12:30 PM Hyatt Regency Orlando, Orlando Ballroom M

Samaneh Farokhirad, Chair Dmitry Kopelevich, Co-Chair

Sponsored by: Transport Processes

**12:30 Paper 47a:** Cryogenic Propellant Transfer Line Chilldown Experiments in 1-g using Low Thermally Conductive Coatings and Pulse Flow — *Jason Hartwig*, *Jacob N. Chung, Samuel Darr*  **12:48 Paper 47b:** Computational Study of 3-Phase Contact Line: Effect of Oscillations on Heat Transfer — *Anisha Pawar, Joel Plawsky* 

**1:06 Paper 47c:** Insulation System Design for Spherical Cryogenic Storage Tanks – *Swapnil Sharma, Mahsa Taghavi, Vemuri Balakotaiah* 

**1:24 Paper 47d:** Hydrodynamics, Conjugate Mass Transfer and Chemical Reaction from a Rising Spherical Droplet — *Hadrien Godé, Sophie Charton, Dominique Legendre, Eric Climent* 

1:42 Paper 47e: Modeling Multicomponent Wax Deposition and Aging on Cold Surfaces with Application to Pipeline Fouling – Samuel Ogunwale, Luqman Ahmad Mahir, Ronald Larson

2:00 Paper 47f: Phenomenological Study of Hazardous Gas Releases from Buried Pipelines — Ola Srour, Konstantinos Kakosimos, Luc Vechot

2:18 Paper 47g: Minimizing Energy Consumption By Insights into Vortex Dynamics in a Fluid Induced By a Freely Rotating Cylinder with Splitter Plate — *Nitin Minocha*, *Chenguang Zhang*, *Rahul Ramaraju*, *Krishnaswamy Nandakumar*, J. B. Joshi

2:36 Paper 47h: The Shear Viscosity of Mixtures Revisited – a Novel Way to Define and Calculate Viscosities for Mixtures and Its Relation to Diffusion – Joe-Hin Yip, Kai Langenbach

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

Tuesday, Nov 7, 12:30 PM Hyatt Regency Orlando, Blue Spring I/II

Dora Lopez De Alonzo, Chair David Miller, Co-Chair Omar Guerra Fernandez, Co-Chair

Sponsored by: Fossil Energy

12:30 Paper 48a: Systematic Comparison of CO<sub>2</sub> Capture Towards the Renewable Production of Methanol and Methane: Spain Case - Guillermo Galán Iglesias, Mariano Martin, Ignacio Grossmann

12:55 Paper 48b: Amine Vapor Emissions Control Technology for Water-Lean Solvents for Point Source CO<sub>2</sub> Capture – Jacob Nelson, Lucas Cody, Moumita Bhattacharya, Paul Mobley, Jak Tanthana, Daniel Mogollon, Addison Lane, Hannah Honeycutt, Marty Lail

**1:20** Paper 48c: Modeling CO2 Adsorption in an Euler-Lagrange Framework Accounting for Pseudo-Turbulence and Intraparticle Diffusion — *Rebecca Grawe*, *Jesse Capecelatro* 

1:45 Paper 48d: Optimizing CO<sub>2</sub> Capture through Solid Adsorption: Developing Optimal Strategies – Ilse María Hernández-Romero, Antonio Flores-Tlacuahuac

2:10: Break

2:35 Paper 48f: Grey and Blue Hydrogen Production Costs in Hydrogen Plants: A Comparative Analysis — *Mary Katebah*, *Mamoun Al-Rawashdeh, Patrick Linke* 

(49) Division Plenary: Valorization of Waste Plastics (Invited Talks)

Tuesday, Nov 7, 12:30 PM Hyatt Regency Orlando, Challenger 41/42

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

**Sponsored by:** Forest and Plant Bioproducts Division

**12:30** Paper 49a: Biocarbon-Metal Sustainable Composites for Energy Storage — *Ange Nzihou* 

**1:00 Paper 49b:** High-Performance Silicon Active Materials from Biorenewable Resources – *Srikanth Pilla* 

1:30 Paper 49c: From Waste to Treasure: Multiple-Functional Materials from Bio-Based Waste – *Zhaohui Tong*  2:00 Paper 49d: Circular Economy Driven Sustainable Composites through Waste Valorisation for Single-Use Plastic Alternatives — Manjusri Misra

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

Tuesday, Nov 7, 12:30 PM Hyatt Regency Orlando, Celebration 9

Matthew Crane, Chair Elizabeth Lee, Co-Chair Peijun Guo, Co-Chair

**Sponsored by:** Electronics and Photonics

12:30: Introductory Remarks

**12:35 Paper 50a:** Dopant Selective Photoelectrochemical Etching of SiC — Samuel J. Whiteley, Adam Sorensen, John J. Vajo, Shanying Cui, **Jason Graetz** 

**1:10** Paper 50b: Modifying Halide Perovskites with Small Molecules for Novel Functionality — *Joseph M. Luther* 

**1:45** Paper 50c: Low Dimensional Metal Halide Perovskites and Hybrids for Optoelectronics — *Biwu Ma* 

2:20 Paper 50d: Let's Twist Again: High-Quality-Factor Metasurfaces to Enhance Spin in Molecules and Monolayer Materials – *Jennifer Dionne* 

(51) Plenary Session for Nanomaterials for Energy Applications (Invited Talks)

Tuesday, Nov 7, 12:30 PM Hyatt Regency Orlando, Discovery 45

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

**Sponsored by:** Nanomaterials for Energy Applications

**12:30 Paper 51a:** Direct Air Capture (DAC) of CO<sub>2</sub> Using Porous Sorbent Materials Coupled with Scalable Processes — *Christopher Jones* 

**1:20 Paper 51b:** Thermally Stable Single Atom Catalysts for Energy Conversion — *Abhaya Datye*  2:10 Paper 51c: Computational Materials Design with Machine Learning and Atomistic Simulations – *Rafael Gomez-Bombarelli* 

(52) Wilson Award Presentation and Lecture (Invited Talks)

Tuesday, Nov 7, 1:30 PM Hyatt Regency Orlando, Atlantic

**Courtney Bottenus, Chair** 

**Sponsored by:** Nuclear Engineering Division

(53) Fluidization: Experimental Investigation and Modeling of Fluidization Processes

Tuesday, Nov 7, 12:30 PM Hyatt Regency Orlando, Bayhill 21

Luke Neal, Chair Eric Jia, Co-Chair

**Sponsored by:** Fluidization and Fluid-Particle Systems

**12:30 Paper 53a:** Dynamical Analysis of Velocity Time Series in a Binary Fluidized BED: MODEL Validation with Radioactive Particle Tracking (RPT) Experiments – *Subi Nath, Akshat Yadav, Shantanu Roy* 

**12:50 Paper 53b:** Novel Pathways for Fluidized Bed Coating with the Aid of Non Conventional Fluidizing Media: Experiments and Models – Aydin Sunol, Anurag Guha

1:10 Paper 53c: Quantifying Powder Cohesivity through Fluidisation Tests – *Amalia Thomas, Nathalie Vriend, Alexander Routh* 

**1:30 Paper 53d:** 100 Years of Scaling up Fluidized Bed and Circulating Fluidized Bed Reactors — **Jia Wei Chew**, Wyatt Casey LaMarche, Ray Cocco

**1:50** Paper 53e: Behaviour of Lumps in Gas-Solid Fluidized-Bed Reactors — *Matteo Errigo*, *Massimiliano Materazzi, Paola Lettieri* 

2:10 Paper 53f: Improving FCC Regenerator Performance and Capacity Utilization through CFD Analysis – *Zhizhong Ding*, Todd Foshee, Manoj Katakdaunde, Robert Ludolph 2:30 Paper 53g: CFD Modeling of Particle Binary Mixing in Fludized Bubbling Bed Reactors - Kuochen Tsai

(54) Experiences in Teaching Process Safety

Tuesday, Nov 7, 12:30 PM Hyatt Regency Orlando, Bayhill 29

Kenneth Cox, Chair Raymond Rooks, Co-Chair Sponsored by: Product Design

**12:30 Paper 54a:** Resources for Teaching Process Safety That Are Managed or Have Been Developed By the Center for Chemical Process Safety — **Bruce Vaughen**, Dr.Anil Gokhale

12:49 Paper 54b: Increasing Chemical Engineering Students' Awareness of New out-of-Textbook Safety Topics — Jack Shultz, Jared Rhodes, Joontaek Park

1:08 Paper 54c: Bringing the Real World into the Classroom: A Risk-Based Assessment of the Train Derailment in East Palestine, Ohio – Obioma Uche

1:27 Paper 54d: Understanding Engineering Students' Approaches to Process Safety Judgements through a Digital Process Safety Game – Cayla Ritz, Brittany Butler, Jeffrey Stransky, Cheryl A. Bodnar, Emily Dringenberg, Elif Miskioglu

1:46 Paper 54e: Teaching Process Safety with Simulink Simulations of Runaway Reactions — Akhil Gopinath, Spandhana Gonuguntla, Aycan Hacioglu

2:05 Paper 54f: Development of an Elective Process Safety Course at the University of Michigan - Kenneth First, Henry Y Wang

2:24 Paper 54g: Instruction of Process Safety Engineering through Project Based Learning (PBL) – Pedro J. Arias-Monje, Sepehr Arbabi

2:43 Paper 54h: On the Use of CSB Videos for Reflective Learning in Teaching Process Safety — Paul Amyotte (55) Honorary Session for Prof. Steve Cramer I (Invited Talks)

Tuesday, Nov 7, 12:30 PM Hyatt Regency Orlando, Coral Spring I/II

Cristiana Boi, Chair Ranil Wickramasinghe, Co-Chair

Sponsored by: Bio Separations

12:30 Paper 55a: Recent Advances and Current Directions in Downstream Processing for Biotherapeutics — Anish Dighe, Vivekananda Bal, Ayse Eren, Dulashani Ruwanthika Ranasinghe Weerakkodige, Jay Yadav, Moo Sun Hong, Paul W. Barone, Stacy Springs, Anthony Sinskey, Allan S. Myerson, **Richard Braatz** 

**12:48 Paper 55b:** Innovation in Downstream Processing: Next Generation Solutions and Need for Speed — *Nihal Tugcu* 

1:06 Paper 55c: Integrated Membrane Process for the Isolation of Plant-Derived Extracellular Vesicles. — Sara Giancaterino, Riccardo Onesti, Cristiana Boi

1:24 Paper 55d: Improving Filtration Performance of Virus Filters at High Product Titers — Wenbo Xu, Xianghong Qian, **Ranil** Wickramasinghe

**1:42** Paper 55e: SMA and ACT: A Tale of Two Isotherms — *Todd Przybycien* 

2:00 Paper 55f: The Effect of Monovalent Cations on the Structure and Dynamics of Multimodal Chromatographic Surfaces – Camille Bilodeau, Emily Baum, Daniel Garzon

2:18 Paper 55g: Scaled-Down, High-Throughput Optimization of Lentiviral Vector Production for Therapeutic and Drug Discovery Applications — Sneha Gopal, Seok-Joon Kwon, Maisha Feroz, Ronit Ghosh, Shivani Kulkarni, Todd Przybycien, Steven Cramer, Jonathan Dordick

**2:36 Paper :** Tissue Adhesive Tattoos for Gastrointestinal Endoscopy — *Kaushal Rege*  (56) Topical Plenary: Environmental Analytical Technology: Sensor Applications in Sustainability (Invited Talks)

Tuesday, Nov 7, 12:30 PM Hyatt Regency Orlando, Celebration 16

Ariel Furst, Chair Stephanie McCalla, Co-Chair

**Sponsored by:** Sensors for Sustainability

12:30: Introductory Remarks

**12:40 Paper 56a:** Invited Talk by Dr. Gang Fan – *Gang Fan* 

1:10 Paper 56b: Invited Talk from Prof. Astrid Mueller — *Astrid Mueller* 

1:40 Paper 56c: Invited Talk from Dr. Bertrand Neyhouse — *Bertrand J. Neyhouse* 

2:10 Paper 56d: Invited Talk by Prof. Fikile Brushett – *Fikile Brushett* 

2:40: Concluding Remarks

#### (57) Plenary Session: Waste Plastics (Invited Talks)

Tuesday, Nov 7, 12:30 PM Hyatt Regency Orlando, Rainbow Spring I/II

Mary Ellen Ternes, Chair Jeffrey Seay, Co-Chair Shelby Browning, Co-Chair

Sponsored by: Waste Plastics

12:30 Paper 57a: Plastic Policy Developments for Chemical Engineers 2023 – *Mary Ellen Ternes* 

1:00 Paper 57b: Scale-Up of PureCycle Solvent Dissolution Recycling Process — *Dustin Olson* 

1:30 Paper 57c: Advanced Recycling Applications around the World – *Shelby Browning* 

2:00 Paper 154af: Polymer-Based Catalyst for Efficient Glycolysis of Poly (ethylene terephthalate) (PET) - Fahimeh Forouzeshfar, Maria Coleman, Joseph Lawrence 2:30 Paper 57e: Revolutionizing Sustainability: TimePlast's Integration of Advanced Computing and Engineering for Water Soluble, Time-Programmable Bioplastics - Manuel Rendon, Tony Martinez, Thomas Anderson, Christina Fontanesi

(58) Interactive Session: Applied Mathematics and Numerical Analysis

Tuesday, Nov 7, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

Joel Paulson, Chair Kamil Khan, Co-Chair

**Sponsored by:** Applied Mathematics and Numerical Analysis

**Poster 58a:** Towards an Integrated Wide Approach for Upstream Field Recovery — **Shakeel Ramjanee** 

Poster 58b: Towards an Integrated Approach for Upstream Recovery — Shakeel Ramjanee

Poster 58c: Analytical Solutions for the Modeling, Optimization, and Control of Microwave-Assisted Freeze Drying — *Prakitr Srisuma, George Barbastathis, Richard D. Braatz* 

Poster 58d: Computational Modeling of Cell Migration in Complex Chemokine Environments — *Kailei Liu*, *Michael B. Dwinell*, *Ashlee Ford Versypt* 

Poster 58e: Simulating Solute Transport through the Kidney Glomerulus Using Febio – Nicholas O. Glover, Ashlee N. Ford Versypt

Poster 58f: An Improved Algorithm for Flux Variability Analysis — Dustin Kenefake, Erick Armingol, Nathan E. Lewis, Efstratios Pistikopoulos

Poster 58g: Using Dynamic Metabolic Modeling to Predict the Transcriptional Regulation of Cuticle Biosynthesis. – Lohani Esterhuizen, Rajib Saha

Poster 58h: A Computational Model of the Interplay of Pancreatic Islet Beta-Cells and Alpha-Cells on the Secretion of Insulin and Glucagon — Aedan Brown, Emmanuel Tzanakakis Poster 58: Stability and Bifurcation Analysis of Natural Convection Effects in Liquid Hydrogen Tank Dual Layered Insulations – Swapnil Sharma, Vemuri Balakotaiah

Poster 58j: Development of an Optimal Maintenance Scheduling Framework for Maintenance 4.0 Applications – *Louis Allen*, *Joshua Aldred, Martha Scattergood, Joan Cordiner* 

Poster 58k: Simulation and Optimization of Gas Based Ammonia Plant Using Advanced Tools of MS Excel – **Bhupen Mehta**, Chandan Kumar Mishra

Poster 58I: A Smart Computing-Based Protocol for Analysis of Certain Classes of Complex Chemical Reactions – Satish Parulekar

Poster 58m: Quantum Algorithms for Optimization over Discrete Variables — *Nicolas Sawaya* 

Poster 58n: Mathematical Modelling of Gene Delivery in Patients with Haemophilia B — *Elnaz Jamili, Amit C. Nathwani, Vivek Dua* 

Poster 580: A Techno-Economic Model and Decision-Making Matrix for Wastewater Biosolids Reuse Application — *Hesan Elfaki*, *Dhabia Al-Mohannadi* 

Poster 58p: Design and Optimization of Hydrogen-Blended Natural Gas Pipeline and Separation Systems – *Shiya Gu, Yachao Dong, Yu Zhuang, Jian Du* 

Poster 58q: An Enhanced Particle Swarm Optimization Employing Quasi-Random Numbers with Application to Efficient Removal of Pfas from Water — *Shiva Kannan, Urmila Diwekar* 

(59) Interactive Session: Data and Information Systems

Tuesday, Nov 7, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

Salvador García-Muñoz, Chair Maria Papathanasiou, Co-Chair

**Sponsored by:** Information Management and Intelligent Systems Poster 59a: Measure This, Not That: Pareto Optimal Trade-Offs between Model-Based Information Content and Measurements Cost (Poster corresponding to plenary presentation) — *Jialu Wang*, *Alexander Dowling* 

Poster 59b: Real-Time Fault Detection Models for Smart Manufacturing: A Case Study with Heat Exchanger Equipment and Innovation Platform – Lucky Yerimah, Mrunal Sontakke, Andreas Rebmann, Sambit Ghosh, Ronald Hedden, B. Wayne Bequette

Poster 59c: Towards an Integrated Approach for Upstream Field Recovery — *Shakeel Ramjanee* 

Poster 59d: Hybrid Bayesian-Based Surrogate Optimization for Sustainable Process Design within Planetary Boundaries – **Sachin** Jog, Daniel Vázquez, Lucas Francisco Dos Santos, Jose A. Caballero, Gonzalo Guillén-Gosálbez

Poster 59e: Probabilistic Lifespan Prediction of Lithium-Ion Batteries Under Varying Operating Protocols Using Gaussian Process Regression – **Seyeong Park**, Jaewook Lee, Jay Hyung Lee

Poster 59f: Automated Synthesis of Hybrid Models for Ionic Separations — Teslim Olayiwola, Luis Briceno-Mena, Tanmay Kulkarni, Christopher Arges, Revati Kumar, Jose A. Romagnoli

Poster 599: Modeling and Predictive Control of Hybrid Dynamical Systems Using Machine Learning Methods – *Cheng Hu, Ming Xiao, Zhe Wu* 

Poster 59h: Smells like AI: Harnessing Machine Learning for Advanced Olfactory Experience Reproduction and Odorant Optimization — Vinicius Viena Santana, Bruno Rodrigues, Sandris Murins, Nadia Shardt, Idelfonso Nogueira

Poster 59i: A Novel Recurrent Neural Network for Hydroprocessing Unit Modeling Using Neural Circuit Policies and Attention-Based Encoder-Decoder - Shu-Bo Yang, Zukui Li Poster 59j: A Parametric Cost Function Approximation Algorithm for Multiscale Decision-Making – Kaiyu Cao, Asha Ramanujam, Can Li

Poster 59k: Data-Driven Linear Predictive Control of Nonlinear Processes Based on the Reduced-Order Koopman Operator – Xuewen Zhang, Minghao Han, Xunyuan Yin

Poster 59I: Modelling of Non-Conventional Streams in the Context of Circular Economy-the Case of Hydrothermal Liquefaction – Antonios Kokosis

Poster 59m: Data Embedding and Hybrid Modeling for Industrial Fluid Catalytic Cracking — *Antonios Kokosis, Dimitrios Blitas* 

Poster 59n: A Graph Attention Network Based Approach for Interpretable and Domain-Aware Modeling of a Wellhead Water Treatment System — Jasmine Sekhon

Poster 590: Development of Algorithms for Mass and Energy Constrained Dynamic Neural Network Models – Angan Mukherjee, Debangsu Bhattacharyya

Poster 59p: Design of Microfluidic Chromatographs through Reinforcement Learning

— **Mohammad Shahab**, Raghunathan Rengaswamy

Poster 59q: A Continuous Learning, Generative Model Pipeline for Kinetic Model Parameter Estimation — *Michael Volk, Shekhar Mishra, Huimin Zhao* 

Poster 59r: Enhancing Multi-Objective Particle Swarm Optimization with the Cluster-Based Approach: Application to Hydrogen Production Process Optimization — **Seokyoung Hong**, Jaewon Lee, Junghwan Kim

Poster 59s: Investigating the Effects of Tunable Experimental Parameters on hiPSC-Cms Maturation Via Clustering Techniques — *Shenbageshwaran Rajendiran*, *Selen Cremaschi*  Poster 59t: Improving Industrial-Scale Bioreactor Performance: Development and Validation of Computationally Efficient Compartment-Based Models Using Real Plant Data – Parth Shah, Joseph Kwon

Poster 59u: Learning Dynamical Process Models Using Plant Data: A Real-World Case Study in the Sustainable Manufacturing of Insulation Products – *Siddharth Prabhu*, *Srinivas Rangarajan*, *Mayuresh Kothare* 

Poster 59w: Automating the Discovery of Reaction Networks for Complex Reaction Systems from Spectroscopic Measurements – Karthik Srinivasan, Vinay Prasad

Poster 59x: Data-Driven Supply Chain Monitoring Based on Canonical Variate Analysis — Jing Wang, Christopher Swartz, Kai Huang

Poster 59y: Optimal Sensor Network Design for Maximizing Net Present Value and Its Application to Corrosion Monitoring in a Power Plant – Chandra Sekhar Somayajula, Debangsu Bhattacharyya, Xingbo Liu, Shanshan Hu

Poster 59z: Combined Use of Recursive Neural Network (RNN), Convolutional Neutral Network (CNN), and Attention Mechanism on Cycling Data of Lithium Ion Battery for Lifespan Prediction – Jaewook Lee, Jay Hyung Lee

Poster 59aa: Adversarial Data in Demand Side Management - *Eike Cramer* 

Poster 59ab: Generalization Error Bounds for Neural Networks Modeling Two-Time-Scale System Dynamics with Application to Model Predictive Control of Nonlinear Processes – Aisha Alnajdi, Atharva Vijay Suryavanshi, Fahim Abdullah, Panagiotis Christofides

Poster 59ac: Control Lyapunov-Barrier Function-Based Safe Reinforcement Learning for Nonlinear Optimal Control — Yujia Wang, Zhe Wu Poster 59ad: Reinforcement Learning (RL)-Based Process Controller Design: An Implementable Approach - Hesam Hassanpour, Xiaonian Wang, Brandon Corbett, Prashant Mhaskar

Poster 59ae: Efficient Hybrid Modeling and Sorption Model Discovery for Non-Linear Advection-Diffusion-Sorption Systems: A Systematic Scientific Machine Learning Approach — Vinicius Viena Santana, Erbet Costa, Carine Rebello, Ana M. Ribeiro, Christopher Rackauckas, Idelfonso Nogueira

Poster 59af: Using Artificial Neural Networks for Real-Time Tuning of PID Controllers — *Tate Bestwick*, *Kyle V. Camarda* 

Poster 59ag: Chemistry-Aware Retrosynthesis and Forward Reaction Prediction Using Smiles Grammar Tree Transformer – Vipul Mann, Kevin Zhang, Venkat Venkatasubramanian

Poster 59ah: Control Invariant Set Enhanced Reinforcement Learning for Process Control: Improved Sampling Efficiency and Guaranteed Stability — Song Bo, Yin Xunyuan, Jinfeng Liu

Poster 59ai: A Comprehensive Decision Making and Networking Facility for the Biorefining Community – *Edlira Kalemi, Franjo Cecelja* 

Poster 59aj: Hybrid Methods for Battery State of Charge Estimation Based on Electrochemical Model – Seunghyeon Oh, Jiyong Kim, II Moon

Poster 59ak: Structure-Based Prediction of Kinase Activation amidst a Varied Mutational Landscape Using Privileged Learning — **Yiming Wang**, Fangping Wan, Zhangtao Chen, Jonathan Nukpezah, Cesar de la Fuente-Nunez, Ravi Radhakrishnan

Poster 59al: Identifying PDAC Diagnostic Biomarkers Utilizing Machine Learning Combined with Genome-Scale Metabolic Modeling – *Tahereh Razmpour*, *Andrea Goertzen, Rajib Saha*  Poster 59am: Self-Optimizing Control Methodology Using Surrogate Models for Complex Systems: A Jupyter-Based Application for Flexible Exploration and Adjustment — Marcilio Maximo, Herbert Teixeira, Antônio Tavernard, Heleno Bispo

Poster 59an: Chemical Substance Diagnosis System Based on Knowledge Inference and Machine Learning for Chemical Exposure Symptoms – *Kangseop Kim*, *Dongil Shin* 

Poster 59ao: Augmented Control Using Reinforcement Learning and Conventional Process Control – Daniel Beahr, Debangsu Bhattacharyya, Douglas A. Allan, Stephen Zitney

Poster 59ap: Intelligent Size Characterization of Granules By Machine Learning Method – Mehrdad Khakbiz, Maryam Rezaeizadeh, Gerardo Callegari, Fernando Muzzio Sr.

Poster 59ar: Designing pH-Temperature Responsive Microgels with Targeted Transition Temperature Using a Novel Partial Least Squares (PLS) Model Inversion Technique — Prashant Mhaskar, Todd Hoare, Seyed Saeid Tayebi

Poster 59as: Prediction of Chemical Toxicity and Exposure Symptoms Based on Knowledge Graph Embedding and Language Models — Young Min Jung, Jinkyung Son, Kangseop Kim, Dongil Shin

Poster 59at: Data-Driven Adaptive Sparse Identification of Time-Varying Nonlinear Dynamics for 2,3-Bdo Distillation Column — Yeongryeol Choi, Bhavana Bhadriraju, Hyungtae Cho, Jongkoo Lim, Il Moon, Joseph Kwon, Junghwan Kim

Poster 59av: Intelligent Robotic Platform for Closed-Loop pH Adjustment of Personal Care Formulations — *Aniket Chitre*, Jayce Cheng, Alexander Pomberger, Kristina Wang, Long Wang, Kedar Hippalgaonkar, Alexei A. Lapkin (60) Interactive Session: Systems and Process Design

Tuesday, Nov 7, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

Selen Cremaschi, Chair David Miller, Co-Chair

**Sponsored by:** Systems and Process Design

Poster 60a: An Optimization Model for the Integration of the Hydraulic Fracturing with a Power Plant Considering CO2 As Fracture Fluid — Victor Osvaldo Vega-Muratalla, Luis Fernando Lira-Barragán, Roberto Guerra-González

Poster 60b: Simultaneous Integration of Machine Learning in a Mixed-Integer Nonlinear Programming Formulation to Optimize Gas Production and Water Management in Shale Gas Reservoirs — Francisco Javier López Flores, Luis Fernando Lira-Barragán, Eusiel Rubio-Castro, Mahmoud El-Halwagi, José María Ponce-Ortega

Poster 60c: Modeling and Simulation of a Process That Converts Ethane to Low Density Polyethylene – Ernest Mokaya, Omar Almaraz, Srinivas Palanki

Poster 60d: Simultaneous Optimization of Electrochemical CO<sub>2</sub> Reduction Process and Reaction System — *Youngwon Lee, Sun Young Lee, Jonggeol Na* 

Poster 60e: Physics-Guided Autonomous Design for Acid-Stable Water Oxidation Catalyst — Areum Han, Yesol Lee, Dong Hyeon Mok, Seoin Back, Young Jin Sa, Jonggeol Na

Poster 60f: Explainable Artificial Intelligence (XAI)-Based Causality Analysis for Chemical Process — Yuna Ko, Kyojin Jang, Jonggeol Na

Poster 60k: Control of the Absorption so<sub>2</sub> with Naoh Solution in Packed Columns Using Aveva Process Simulation — Paulo Henrique N. Ferreira, Carlos Alexandre M. da Silva, **Milene** Codolo Poster 60I: Heuristic-Aided Emulgels Design for Food and Cosmetic Applications — Natalia Linares, Juan Sebastian Rodríguez, Javier Camilo Martínez, Alvaro Orjuela, Rolando Acosta, Camilo Andrés Castro

Poster 60m: Analysis of Correlation between Microbubble and Precipitated Calcium Carbonate Size Using Image Processing Model for Carbon Utilization Process – Yup Yoo, Yujeong Yun, Youngbok Ryu, Hojun Song, Hyun Sic Park, Junghwan Kim, Hyungtae Cho

Poster 60n: An Energy Efficient Process Design for Ethyl Levulinate Production Using Double Reactive Distillation Columns – **Devrim Kaymak**, Aslihan Balkan

Poster 60o: Process Development and Analyses for Production of Green Hydrogen Using Liquefied Natural Gas Cold Energy – *Bomin Choe, Wangyun Won* 

Poster 60p: A Novel Carbon Emission Optimization Method for Chemical Processes Based on Thermodynamic 1st and 2nd Law: Naphtha Cracking Center Application — *Wonjun NOH*, *Juyeong SEO*, *Seoyeon CHO*, *Inkyu Lee* 

Poster 60q: Multiscale Modeling of Dry Reforming of Methane to Study the Effect of Catalyst Morphology – *Hye Min Choi*, *Joseph Kwon, Jay Hyung Lee* 

Poster 60r: A Hybrid Catalytic Route to Ethanol from Residue Gases Via the Dimethyl Ether and Methyl Acetate Synthesis: Process Design and Techno-Economic Analysis – *Minseong Park*, *Chanhee You, Chanmok Kim, Hyeon Yang, Thai Ngan Do, Jiyong Kim* 

Poster 60s: Synthesis of Indirect Multi-Plant Heat-Integrated Water Allocation Networks – Jack Chou, Linlin Liu, Jian Du

Poster 60v: Study of CO2 Absorption in Packed Columns Using Aveva Process Simulation - Vinicius S. S. Machado, Carlos Alexandre M. da Silva, **Milene** Codolo (61) Interactive Session: Systems and Process Operations

Tuesday, Nov 7, 3:30 PM Hyatt Regency Orlando,

Regency Ballroom R/S Faruque Hasan, Chair Qi Zhang, Co-Chair

**Sponsored by:** Systems and Process Operations

Poster 61a: Decision-Focused Surrogate Modeling for Mixed-Integer Optimization (Poster corresponding to plenary presentation) — *Shivi Dixit, Rishabh Gupta, Qi Zhang* 

Poster 61b: Neural Network Models for Predicting Impurity Removal Amount in ARDS Process and Operation Condition Optimization Using Genetic Algorithm — Yungun Jung, Yeonsoo Kim

Poster 61c: Simulation and Optimization of the Supply-Chain of Plastic Recycling with Environmental Considerations — *Elisavet Anglou*, *Riddhi Bhattacharya*, *Patritsia M. Stathatou*, *Fani Boukouvala* 

Poster 61d: Temporal Intergrated Planning of Design, Shipping Scheduling, and Energy Management System for International Hydrogen Supply Chain — Jay Hyung Lee, Sunwoo Kim

Poster 61e: Reliable Design and Optimization of Crystallization Systems Under Uncertainty – Yash Barhate, Zoltan Nagy

Poster 61f: Applying a Comprehensive View of Resilience to Power Distribution Network Optimization — **Benjamin P. Riley**, Prodromos Daoutidis, Qi Zhang

Poster 61g: Adjustable Robust Optimization for the Synthesis of Continuous Rufinamide Manufacturing Process Under Uncertainty – *Wenhui Yang*, *Taoyu Qiu, Zhihong Yuan* 

Poster 61h: Integrated Design and NMPC-Based Control Under Uncertainty and Naturally Ordered Structural Decisions: A Discrete-Steepest Descent Approach. — Oscar Palma-Flores, Luis Ricardez-Sandoval, Lorenz Biegler Poster 61i: Uncertainty Quantification of Physics Informed Neural Networks Using Bayesian-Last-Layer Approach, and Its Application to Real-World Bioprocess – Shu Yang, Huiyi Cao, William Fahey, Reza Kamyar

Poster 61k: A Framework for Resilient Multi-Product Supply Chains: An Application to Healthcare – *Miriam Sarkis*, *Nilay Shah, Maria Papathanasiou* 

Poster 61I: Reducing Solution Times of Continuous Production Scheduling MILP Models with Record Keeping Variables – Amin Samadi, Christos T. Maravelias

Poster 61m: Perspective Reformulation of Stochastic Agrochemical Supply Chain Optimization Problem with Mean-Variance Risk Management – Saba Ghasemi Naraghi, Zheyu Jiang

Poster 61n: Integration of Production Planning and Scheduling Problems with Uncertainty and Feasibility Analysis – *Ziqing Guo*, Yachao Dong, Jingxing Gao, Jian Du

Poster 61o: Multi-Stage Stochastic Programming for the Planning of a Mobile Modular Closed-Loop Supply Chain – Congqin Ge, Zhang Lifeng, Wenhui Yang, Zhihong Yuan

Poster 61p: Energy Flow Redistribution for Optimal Operation of Heat Exchanger Networks — *Karthika Mohanan, Sujit Jogwar* 

Poster 61q: Management of Multi-Microgrid System with 2D CNN Forecasting Model and End-Effect Mitigation Using Value Function – Dongho Han, Teemu Ikonen, liro Harjunkoski, Jay Hyung Lee, Seongmin Heo

Poster 61r: Clustering-Based Forecasting Framework for the Energy Sector – *Funda Iseri*, *Harsh Shah, Rahul Kakodkar, Efstratios Pistikopoulos* 

Poster 61s: Applications of Data-Driven Approaches in Chemical Process and Energy System Optimization — *Mohammed Alkatheri*, *Tuhin Poddar*, *Ali Elkamel*, *Ali Almansoori*  Poster 61t: Use of Bayesian Optimization for Efficient Finding of Optimal Operating Condition of Simulated Moving Bed Process - Woohyun Jeong, Jay Hyung Lee

Poster 61u: Optimization of Waste Water Plant Operations — *Komal Rathore*, *Aydin Sunol, Tolga Pirasaci, Andres Tejada-Martinez, Kiesha Pierre, Aaron Driscoll, Gita Iranipour, Kyle Cogswell* 

Poster 61v: Quantitative Studies of Decomposition Algorithm Efficiencies for Global Nonconvex Stochastic Optimization Problems – Pengfei Cheng, Joseph K. Scott

Poster 61w: Accelerating Process Design and Optimization with Novel Computational Tools — Patrik Furda, Juraj Myšiak, Miroslav Variny

Poster 61x: Generalised Optimisation Framework for Process Synthesis and Intensification in the Equation-Oriented Environment – Chao Liu, Yingjie Ma, Dongda Zhang, Jie Li

Poster 61y: Learning to Select the Best Optimization Solution Strategy: An Algorithm Selection Approach — *Ilias Mitrai*, *Prodromos Daoutidis* 

Poster 61z: Stochastic Community Detection: Novel Solution Approach and Application to Sustainable Process Operations — Hongxuan Wang, Andrew Allman

Poster 61aa: Adaptive Real-Time Exploration and Optimization for Safety-Critical Industrial Systems: The Arteo Algorithm — Buse Sibel Korkmaz, Tong Liu, Marta Zagorowska, Mehmet Mercangoz

Poster 61ab: A Comparison of Nonlinear Optimal Control Trajectory Sensitivity Formulations - Hainan Wang, Edward Gatzke

Poster 61ac: Discrete Nonlinear Optimization: Modeling and Solutions Via Novel Hardware and Decomposition Algorithms – David E. Bernal Neira (62) Collaborative Discussion: Empathy in Action - Catalyzing Inclusivity for LBGT+ and Marginalized Communities in ChemE

Tuesday, Nov 7, 3:30 PM Hyatt Regency Orlando, Bayhill 31

### Alon McCormick, Chair

Sponsored by: LGBTQ+ and Allies Community

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

Tuesday, Nov 7, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

Gaurav Giri, Chair Rachel Letteri, Co-Chair Kelly Burke, Co-Chair

Sponsored by: Inorganic Materials

Poster 63a: Pathway to Develop a Carbonate-Based Protective Layer in Zinc Ion Batteries — *Anuja Tripathi* 

Poster 63b: Rhenium-Tungsten Alloy Feedstock Preparation Using Incipient Wetness Impregnation — Davis R. Conklin, Hermann Klein-Hessling Barrientos, Alan Weimer

Poster 63d: Effect of Wool Substrate and Its Processing on the Performance of Conductive Textiles – *Alyssa Grube*, Syed Ibrahim Gnani Peer Mohamed, Laurel Hilger, Mona Bavarian

Poster 63e: Material Properties of Recycled Glass Sand: A Case Study Conducted with Glass Half Full Nola – Julie Albert, Julie Vanegas, Nicholas Borne, Shehbaz Ahmad, Leah Michaeloff, Diego Molina

Poster 63f: Unlocking Kinetically-Limited Nucleation Regimes through Continuous Modular Microfluidics – *Jacob Crislip*, *Andrew R Teixeira* 

Poster 63g: In Situ Characterization of Zeolite Surface Growth Using Atomic Force Microscopy – *Zhiyin Niu*, *Rishabh Jain, Madhuresh Choudhary, Jeffrey Rimer*  Poster 63h: Elucidating the Mechanism of Nanosheet Pillaring in MFI-Type Zeolites

— **Muhammad Fiji Firdaus**, Tanvir Ahmed, Rishabh Jain, Luke Tufaro, Patrick Kruszon-Oeffner, Simon Vornholt, Karena Chapman, Jeffrey Rimer

Poster 63i: A Priori Data Collection for Thermodynamic Modeling of Off-Stoichiometric Metal Oxides Via Bayesian Methods – Steven Wilson, Christopher L. Muhich

Poster 63j: Preparation of Two-Dimensional Fe<sub>3</sub>O<sub>4</sub> Nanoparticles Transformed from a-Fe<sub>2</sub>O<sub>3</sub> Analogues and Their Applications in Magnetic Field-Assisted Microalgal Biorefinery Process — **Yujeong Jeong**, Bolam Kim, Laxmi Priya Sathiya Vahisan, Rendi Mahadi, Kyubeom Lee, Eun-Hye Jang, You-Kwan Oh, Sungwook Chung

Poster 63k: Autonomous Synthesis of Eco-Friendly Metal Halide Perovskite Nanocrystals — *Sina Sadeghi, Fazel Bateni, Milad Abolhasani* 

Poster 63I: A Pyrogallate-Based Metal-Organic Framework with a Two-Dimensional Secondary Building Unit — **Stavroula Kampouri**, Mircea Dincă

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

Tuesday, Nov 7, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

Mohammad Hassan, Chair Albert Liu, Co-Chair Ali Alshami, Co-Chair Rachel Letteri, Co-Chair Kelly Burke, Co-Chair

Sponsored by: Composites

Poster 64a: From Brown Tides to 3D Printers: Fabrication & Characterization of Novel Sargassum-Based Polymer Composite Filaments for 3D Printing — Zuanichi Figueroa, Abraham Polanco, Jeziel Rodriguez, Sebastian Toro Bernal, Omar Movil Poster 64b: An Exploratory Study on the Development of Sargassum Algae-Based Biodegradable Polymer Composites Via Selective Laser Sintering. — *Stephanie Garcia, Marielisa Ortiz, Omar Movil* 

Poster 64c: Liquid Metal Polymer Composites to Enable Soft Robotics and Stretchable Electronics – **Amanda Koh**, Anh Hoang, Elizabeth Bury

Poster 64d: Engineering Magnetic Composites for Improved Shear Behavior through Orthogonal Means – *Amanda Koh*, Sandhiya Thiagarajan, Emmanual Johnson

Poster 64e: Prediction of Organic Compound Aqueous Solubility Using Interpretable Machine Learning-a Comparison Study of Descriptor-Based and Topological Models — **Arash Tayyebi**, Ali Alshami

Poster 64f: Sustainable Generator and in-Situ Monitor Forreactive Oxygen Species Using Photodynamic Effect Ofsingle-Walled Carbon Nanotubes in Ionic Liquids — *Erin Witherspoon, Zhe Wang* 

Poster 64g: Highly Stretchable P3HT Containing Core-Shell Composite Fibers from Coaxial Electrospinning — *Humayun Ahmad*, *Maggie Britton, Santanu Kundu* 

Poster 64j: Development of a Novel PEO-Based Solid Electrolyte for Lithium-Sulfur Batteries — Basem Al Alwan, Zhao Wang, Wissam Fawaz, K.Y. Simon Ng

(65) Poster Session: General Topics on Separations

Tuesday, Nov 7, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

**Sponsored by:** General Topics and Other Methods

Poster 65a: Hollow Fiber Membrane Module Fabrication for the Separation of R-410A – Luke Wallisch, Abby Harders, Mark B. Shiflett

Poster 65b: Process-Based Solvent Screening for Efficient Extractive Distillation – Sahil Sethi, Xiang Zhang, Kai Sundmacher Poster 65c: Poster: Real-Time Induced Magnetic Vibration to Reduce Membrane Fouling: Experimental and Modeling Investigation — Jasneet Pala, Ryan Tracy, Milad Esfahani, Nima Mahmoodi

Poster 65d: "Highly Charged Ion-Exchange Membranes for Treatment of Highly Impaired Waters Via Electrodialysis" — Carolina Espinoza, José Carlos Díaz, David Kitto, Hyunjik Kim, Jovan Kamcev

Poster 65e: Investigating Reactive Oxygen Species of Chitosan-Graphene Oxide Composites for Water Treatment Membranes — Justin Puhnaty, Chris Griggs, Audie Thompson

Poster 65f: Numerical Simulations with Continuous Flow in Magnetic Separator — *Hyeon Choe*, Jacob Strayer, Xian Wu, Jenifer Gomez Pastora, Jeffrey Chalmers

Poster 65g: Unexpectedly High Propylene-Selective Mixed-Matrix Membranes with Additive-Incorporated Facile *in-Situ* ZIF-8 Filler Formation Process – Yinying Hua, Hae-Kwon Jeong

Poster 65h: Effect of Capping Group Binding on Chemical Reactivity – *Chinmay Mhatre, Bradley Gibbons, Amanda J. Morris, Karl Johnson* 

(66) Division Plenary: Food, Pharmaceutical, and Bioengineering Division (Invited Talks)

Tuesday, Nov 7, 3:30 PM Hyatt Regency Orlando, Regency Ballroom P

Mark Brynildsen, Chair Whitney Stoppel, Co-Chair

**Sponsored by:** Food, Pharmaceutical & Bioengineering Division

**3:30** Paper 66a: Division 15 Plenary Award - Development of a Microneedle Patch for Long-Acting Contraception – *Mark Prausnitz* 

**4:20 Paper 66b:** Division 15 Early Career Award - Environmental Microbes for Efficient (re)Use of Renewable Feedstocks and Consumer Wastes in Biomanufacturing – *Kevin Solomon*  **4:45** Paper 66c: Area 15A Plenary Award - Engineering of Aromatic Amino Acid Production in Cyanobacteria — *John Morgan* 

5:10 Paper 66d: Area 15C Plenary Award - Data Driven Microbial Strain Engineering — *Ian Wheeldon* 

5:35 Paper 66e: Area 15DE Plenary Award - a Trip to the Zoo: Lessons for Tissue Engineers — Celeste Nelson

(67) AIChE Journal Futures: New Directions in Chemical Engineering Research (Invited Talks)

Tuesday, Nov 7, 3:30 PM Hyatt Regency Orlando, Manatee Spring I

**David Sholl, Chair** 

**Sponsored by:** Publication Committee

**3:30 Paper 67a:** Engineering *Vibrio natriegens* for Degrading and Assimilating Poly(ethylene terephthalate) — *Tianyu Li*, *Stefano Menegatti*, **Nathan Crook** 

**3:49 Paper 67b:** Applications of Lignin-derived Deep Eutectic Solvents in Biorefinery Processes – **Chang Geun Yoo**, Yunxuan Wang, Jiae Ryu, Kwang Ho Kim, Xianzhi Meng, Yunqiao Pu, Yang Tian, Aymerick Eudes, Gyu Leem, Arthur Ragauskas

**4:08** Paper 67c: Predicting Thermodynamic and Transport Properties of Organophosphates: A Molecular Simulation Substitute for Experiments that You Don't Want to Perform — *Gennady Gor, Ella Ivanova* 

**4:27 Paper 67d:** Leveraging multiplex genome engineering and metabolic pathway design to upcycle waste plastics and biomass via aldehyde transformations in live bacteria *— Aditya Kunjapur* 

**4:46 Paper 67e:** Surface Anisotropic Particles, Capillary Interactions, and Dynamics of Fluid Interfaces — *Elton Lima Correia,* **Sepideh Razavi**  5:05 Paper 67f: Designing better drug delivery particles: Protein corona formation and multicomponent aggregation of particles in blood plasma — Aida Lopez Ruiz, Guangliang Liu, Kathleen McEnnis

**5:24 Paper 67g:** AIChE Journal Futures Placeholder 7

5:43 Paper 67h: Stability and kinetics of Fe-based MOFs with diverse structures in aqueous pollutant degradation — Samuel C. Moore, Michele Sarazen

(68) Advances in Life Cycle Assessment

Tuesday, Nov 7, 3:30 PM Hyatt Regency Orlando, Regency Ballroom U

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

**Sponsored by:** Sustainability Science and Engineering

**3:30 Paper 68a:** Study on Life Cycle Assessment and Optimization of Pesticide Production Process from the Perspective of Sustainable Development — *Kexuan Yang* 

**3:50 Paper 68b:** Life-Cycle Assessment Integration into Scalable Open-Source Numerical Models (LiAISON) for Prospective Impact Analysis of Novel Technologies – **Tapajyoti Ghosh**, *Patrick Lamers, Alberta Carpenter* 

**4:10** Paper 68c: Guiding Food Colorant Production Via Fermentation Using Techno-Economic, Life Cycle and Absolute Sustainability Assessment - Samir Meramo, Sumesh Sukumara, Peter Fantke, Eleonora Passuto

4:30 Paper 68d: Community-Engaged Life Cycle Analysis: Ensuring Sustainability While Protecting Sovereignty - Margaret O'Connell, Jenna Trost, Kimberly Marion Suiseeya, Jennifer Dunn

4:50 Paper 68e: On the Interplay of Food Packaging Design and Food Supply Chain Sustainability – Aurora Del Carmen Munguia Lopez, Paola Alejandra Munoz Briones, Styliani Avraamidou, Victor Zavala (69) Advances in smart monitoring, optimization and control of process manufacturing

Tuesday, Nov 7, 3:30 PM Hyatt Regency Orlando, Bayhill 32

Zhenyu Wang, Chair Masoud Soroush, Co-Chair

Sponsored by: Digital Manufacturing

3:30 Paper 69a: Designing Efficient Human-Machine Interfaces for Decision-Support Tools: Case Studies in Healthcare and Process Systems – *Mrunal Sontakke*, *Sambit Ghosh*, *Faye Cameron, Alan Ganz, Henry Weber*, *Lucky E. Yerimah, Andreas Rebmann, Craig Dory, Ronald Hedden, Joel Plawsky, Johnson Samuel, B. Wayne Bequette* 

**3:49 Paper 69b:** GMP Implementation of Continuous Manufacturing: A Case Study - Edward Wong

**4:08 Paper 59v:** Machine Learning-Based Prediction and Optimization of Liquid Wettability of an iCVD-Produced Fluoropolymer — Daniel Schwartz, Tien Nguyen, Zhengtao Chen, Kenneth Lau, Michael C. Grady, Ali Shokoufandeh, **Masoud Soroush** 

**4:27 Paper 69d:** Towards Scalable and Cost-Effective Plasmid DNA Manufacturing — *Niki Triantafyllou*, *Miriam Sarkis*, *Nilay Shah*, *Maria Papathanasiou*, *Cleo Kontoravdi* 

**4:46 Paper 69e:** Barrier-Free Paper Analytical Devices for Multiplex Colorimetric Detection — *Ayushi Chauhan, Bhushan J. Toley* 

5:05 Paper 69f: Advanced Manufacturing Via Self-Assembled Colloidal Cracking of Binary Nanoparticles — *Ryan Dumont, Bo Li* 

5:24 Paper 699: Bioprocess Control Using Stoichiometric Models of Metabolism — *Mariana Monteiro*, *Sarah Fadda*, *Cleo Kontoravdi*  **5:43 Paper 69h:** Edge-Enabled Monitoring System in 3D Printing Manufacturing Factory — *Michelle C. Almendrala, Danielle Jaye Agron* 

(70) Department Heads Forum (Invited Talks)

Wednesday, Nov 8, 8:00 AM Hyatt Regency Orlando, Bayhill 22

Daniel Shantz, Chair C. Heath Turner, Co-Chair

**Sponsored by:** Department Heads Forum

8:00: Introductory Remarks

8:05 Paper 70a: Salary Survey – *Tyler Johannes* 

8:35 Paper 70b: ABET Update – Randy S. Lewis

8:45 Paper 70c: State of the Institute – Darlene Schuster

9:15: Panel Discussion

9:45: Open discussion

10:25: Concluding Remarks

(71) Atmospheric Chemistry and Physics: Laboratory, Modeling, and Field Studies

Wednesday, Nov 8, 8:00 AM Hyatt Regency Orlando, Silver Spring I/II

Marwa El-Sayed, Chair Coty Jen, Co-Chair

Sponsored by: Air

8:00 Paper 71a: Strategies to Understand Dust Transport and Screen for Potential Health Impacts – Kamaljeet Kaur, Reuben Attah, Kerry Kelly

8:20 Paper 71b: Observations of Atmospheric Conditions during the 2020 Solar Eclipse over South America – Konstantine Geranios, Alexander Chambers, Malachi Mooney-Rivkin, Jennifer Fowler, Matthew Bernards

8:40 Paper 71c: COSMO-RS Re-Parameterization for Accurately Predicting Deep Eutectic Solvent-Fluorinated Compound Systems. — *Thomas Quaid, Toufig Reza*  **9:00 Paper 71d:** Rapid Photolysis Decay of Gaseous Organic Nitrates Formed from Hydroxyl and Nitrate Radical Oxidations of  $\alpha$ -Pinene and  $\beta$ -Pinene – **Nga Lee Ng**, *Masayuki Takeuchi, Yuchen Wang* 

9:20 Paper 71e: PM<sub>2.5</sub> bound Species Variation and Source Characterization in the Post-Lockdown Period of the Covid-19 Pandemic and Fireworks Period in National Capital of India – *Mohd Faisal, Umer Ali, Vikram Singh, Mayank Kumar* 

9:40 Paper 71f: Eliminating Soot Emissions from Jet Fuel Combustion – *Georgios Kelesidis*, Amogh Nagarkar, Una Trivanovic, Sotiris E. Pratsinis

**10:00 Paper 71g:** "I Can't Breathe:" the Invisible Slow Violence of Breathing Politics in Minneapolis – *Marwa El-Sayed*, *Heather O'Leary, Scott Parr, Deondre Smiles* 

**10:20 Paper 71h:** Development of Large-Scale Fire Whirls for Offshore Oil Spill Cleaning — *Mitchell Huffman, Joseph Dowling, Bhushan Pawar, Wuquan Cui, Mohammadhadi Hajilou, Karen Stone, Elaine Oran, Michael J. Gollner, Qingsheng Wang* 

(72) Division Plenary: Materials Engineering & Sciences Division (Invited Talks)

Wednesday, Nov 8, 8:00 AM Hyatt Regency Orlando, Celebration 5

April Kloxin, Chair Rafael Verduzco, Co-Chair Adrianne Rosales, Co-Chair

**Sponsored by:** Materials Engineering and Sciences Division

8:00 Paper 72a: Braskem Award Lecture: Ion Solubility, Diffusivity, and Transport in Charged Polymer Membranes — *Benny D. Freeman* 

8:30 Paper 72b: Owens Corning Early Career Award Lecture: Supramolecular Design of Biomaterials and Drug Delivery Technologies – *Matthew Webber* 

**9:00 Paper 72c:** Organic Electronics and Optoelectronics: Enabling New Energy and Information Technologies - Samson A. Jenekhe 9:30 Paper 72d: Peering into Batteries: Insights into Electrochemical Behavior through Operando and in-Situ Characterization — Esther Takeuchi, Amy C. Marschilok, Kenneth J. Takeuchi

10:00 Paper 72e: Bio-like Soft Materials with Life-like Intelligence - Ximin He

(73) Functional Nanoparticles and Nanocomposites

Wednesday, Nov 8, 8:00 AM Hyatt Regency Orlando, Bayhill 21

Jaewon Lee, Chair

Sponsored by: Nanoparticles

8:00 Paper 73a: Polymer-Grafted Plasmonic Nanocomposites with Enhanced Chiroptical Properties — Shema Rachel Abraham, Jojo P. Joseph, Alexander Baev, Paras N. Prasad, Mark Swihart

8:18 Paper 73b: Preceramic Polymer Grafted Nanoparticle Composites: Influence of Thermal Curing on Rheology, Microstructure, and Ceramic Yield – Gary Germanton Jr., Pitchaimari Gnanasekar, Subramanian Ramakrishnan

8:36 Paper 73c: Perovskite-Coated Biomimetic Chiral Microparticles with Circularly Polarized Light Emission – Michael Veksler, Nicholas Kotov

#### 8:54: Break

9:12 Paper 73e: Electrically Responsive Yolk-Shell Colloidal Photonic Crystals with Controllable Coherent Scattering Intensities — Hikaru Namigata, Tom A. J. Welling, Kanako Watanabe, Keishi Suga, Arnout Imhof, Alfons van Blaaderen, Daisuke Nagao

9:30 Paper 73f: Essential Oil-Loaded Mesoporous Silica Nanoparticles for the Development of Multifunctional Nonfouling Coatings — *Minchen Mu*, Yu-Ting Lin, William DeFlorio, Yashwanth Arcot, Shuhao Liu, Wentao Zhou, Xunhao Wang, Younjin Min, Luis Cisneros-Zevallos, Mustafa Akbulut 9:48 Paper 73g: Silica-Polyelectrolyte Nanocomposites As Stabilizers for Aqueous Microcapsules with Adjustable Properties — *Matthew Lertola*, *Michael B. Schmithorst, Michael Persson, Romain Bordes, Krister Holmberg, Bradley F. Chmelka* 

# (74) Particle Breakage

Wednesday, Nov 8, 8:00 AM Hyatt Regency Orlando, Bayhill 19

Jung-Sheng Wu, Chair Priscilla Hill, Co-Chair

**Sponsored by:** Particle Production and Characterization

8:00: Delayed Start

8:40 Paper 74b: Breakage Kernels Based on 2D Analysis of High Aspect Ratio Particles — *Priscilla Hill* 

9:00 Paper 74c: Bridging Crystallization and Mechanical Properties to Particle Size Reduction Efficiency in Jet Milling Industrial Pharmaceutical Processes – Goncalo Marcelo, André Dias, Luis Sobral, Rachid Santos, João Sequeira, Tiago Porfirio

**9:20 Paper 74d:** Breakage of Alumina Aggregates Under Shear By CFD-DEM Simulations – *Eirini Goudeli, Lequan Zeng, George Franks* 

9:40 Paper 74e: Comminution of Carbon Particles in a Fluidized Bed Reactor: A Review — Sama Manzoor, Erin Bobicki

**10:00 Paper 74f:** Buckling of a Particles Suspension Drop during Fast Drying: Experiments — **Om Prakash Bamboriya**, Mahesh Tirumkudulu

(75) Division Plenary: Pharmaceutical Discovery, Development, and Manufacturing Forum (Invited Talks)

Wednesday, Nov 8, 8:00 AM Hyatt Regency Orlando, Regency Ballroom Q

Kevin Seibert, Chair Carla Luciani, Co-Chair Christopher Marton, Co-Chair

**Sponsored by:** Pharmaceutical Discovery, Development and Manufacturing Forum

8:00 Paper 75a: PD2M Plenary 1 - Andrew Livingston

8:50 Paper 75b: PD2M Plenary 2 — Paresma Patel

9:40 Paper 75c: PD2M Plenary 3 – Eleni Dokou

(76) Challenges and Best Practices in Technology Commercialization I

Wednesday, Nov 8, 8:00 AM Hyatt Regency Orlando, Bayhill 27

John Peragine, Chair Raymond Rooks, Co-Chair Ha Dinh, Co-Chair

**Sponsored by:** Technology Transfer and Manufacturing

8:00 Paper 76a: Utilizing Digital Transformation to Accelerate Technology Commercialization — Anam Ahmed

8:30 Paper 76b: Modular Process Development (versus Designing Modular Process Equipment) - Robert Nunley

**9:00** Paper 76c: Characterization of Non-Traditional Reactors for Scale up of Highly Branched Polymers – *Jennifer Larimer* 

9:30 Paper 76d: Multiphase Reaction/Separation Processes; Technologies and Apparatus Design — Georg Rudelstorfer, Rafaela Greil, Dominik Wickenhauser, Maximilian Neubauer, Matthäus Siebenhofer, Susanne Lux, Annika Grafschafter

(77) John M. Prausnitz AIChE Institute Lecture

Wednesday, Nov 8, 11:15 AM Hyatt Regency Orlando, Plaza International Ballroom G/H

Yu Shi, Chair Martha Grover, Co-Chair

Sponsored by: Awards Committee

11:15 Paper 77a: Translation of Biomedical Microtechnologies from the Lab to the Clinic – Mark Prausnitz (78) ABET Updates and Insights (Invited Talks)

Wednesday, Nov 8, 12:30 PM Hyatt Regency Orlando, Bayhill 22

**Thomas Spicer III, Chair** 

**Sponsored by:** Undergraduate Education

#### (79) Advanced Treatment Technologies for Water I

Wednesday, Nov 8, 12:30 PM Hyatt Regency Orlando, Blue Spring I/II

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

#### Sponsored by: Water

**12:30 Paper 79a:** Superfine Activated Carbon-Functionalized Adsorptive Thin-Film Nanocomposite Membranes for Selective Pfas Removal from Water — *Medha Kasula, Jasneet Pala, Milad Esfahani* 

**12:49 Paper 79b:** Development of Cationic Hydrogel PAC Composites for Pfas Remediation in Aqueous Solutions — *Maria Victoria Ximenes Klaus, Nicole Marguerite, J. Zach Hilt* 

1:08 Paper 79c: Photocatalytic Removal of Heavy Metals from Private Well Water — *Liz Diaz*, *Kevin McPeak* 

**1:27 Paper 79d:** The Role of Redox-Active Metallopolymers in the Selective Remediation of Water from Pfas Contaminants — **Paola Baldaguez Medina**, Valentina Ardila Contreras, Johannes Elbert, Markus Gallei, Xiao Su

**1:46 Paper 79e:** Two-Dimensional Molybdenum Disulfide Based Field Effect Transistor Sensor for Pfas Detection in Water — *Md Mohidul Alam Sabuj, Mo Li, Maria Armanious, Meng-Qiang Zhao* 

2:05 Paper 79f: Polyelectrolyte Nanofiltration Membranes for Base Recovery Processes – Joshua Livingston, G. Kane Jennings, Shihong Lin **2:24 Paper 79g:** Evaluation of a Janus Membrane for Enhanced Rejection of PFAS in Membrane Distillation — *Hyunsik Kim*, *Mallikarjuna Nadagouda, Tae Lee* 

2:43 Paper 79h: Graphene As a Rational Interface for Enhanced Removal of Cyanotoxins and Emerging Contaminants for Water Security – Jesse Roberts, Sarah Grace Zetterholm, Luke A. Gurtowski, Ashvin Fernando, Kevin Wyss, Angela Evans, Justin Puhnaty, Brianna Fernando, Audie Thompson, James M. Tour, Chris Griggs

(80) CO2 Industrial, Engineering and R&D Approaches

Wednesday, Nov 8, 12:30 PM Hyatt Regency Orlando, Silver Spring I/II

Selen Cremaschi, Chair Xiaonan Wang, Co-Chair

Sponsored by: Sustainability

**12:30 Paper 80a:** The Feasibility of Palm-Based Biomass Co-Firing and Different Oxygen Carriers to Enhance the Performance of Coal-Based IGCC Power Plant – *Nasir Al Lagtah* 

**12:48 Paper 80b:** Process Modeling, Techno-Economic and Life-Cycle Assessments of Producing Potentially Carbon-Negative Building Material from CO<sub>2</sub> and Waste Lignin or Lignite - **Yuan Jiang**, Francesca

Pierobon, Nicholas Nelson, Keerti Kappagantula, Satish Nune, David J. Heldebrant

**1:06 Paper 80c:** Improved Approach for Benefit Analysis of Carbon Dioxide Reduction Methods That Use Rechargeable Batteries – *Leisa Porter, Robert Deshotels* 

**1:24 Paper 80d:** Evaluating on-Board CO<sub>2</sub> Capturing Methods for the Ship with Outlook on Storage and Utilization Options — *Mamoun Al-Rawashdeh*, *Jaafar Ballout, Dhabia Al-Mohannadi, Gareth Burton, Joseph* 

Rousseau, Patrick Linke

1:42 Paper 80e: A Cross-Sector Tool for Assessing and Strategizing Mitigation of Industrial Carbon Dioxide Emissions — Ajay Koushik V, Ram Kishore Sankaralingam, Peter Kamau Waiyaki, Achyuta Krishnan, Arun Muthukkumaran, Ramesh Murugan Natarajan, Gowri Shankar Navagana, Satyanarayanan Seshadri, Preeti Aghalayam, **Raghunathan Rengaswamy** 

2:00 Paper 80f: A Framework for the Combined Evaluation of Economic and CO<sub>2</sub> Fixation Feasibility of Carbon Capture and Utilization (CCU) Reaction Pathways – Gasim Ibrahim, Mohamed Sufiyan Challiwala, Mahmoud El-Halwagi, Nimir Elbashir

2:18 Paper 80g: Determination of CO<sub>2</sub> Solubility in Brines and Hydrocarbons for Carbon Storage and Enhanced Oil Recovery - Sushobhan Pradhan, Rupom Bhattacherjee, Clint Aichele, Prem Bikkina

**2:36 Paper 80h:** Research on the Construction of Advanced CO<sub>2</sub> Capture Absorbent and the Regeneration Enhancement Strategy – *Weixin Kong* 

(81) Emerging Junior Investigator Open Innovation Forum (Invited Talks)

Wednesday, Nov 8, 12:30 PM Hyatt Regency Orlando, Celebration 6

Dongjin Seo, Chair Hyun-Tae Hwang, Co-Chair Taeyoung Kim, Co-Chair Won Tae Choi, Co-Chair

**Sponsored by:** International Committee

12:30 Paper 81a: Beyond Surface Facilitates Electrocatalytic Reactions of Renewable Carbons – Dohyung Kim

**12:55 Paper 81b:** Rationally Designing Nanoporous Catalytic Materials for Sustainable Energy Applications — *Hong Je Cho* 

**1:20 Paper 81c:** Nanoparticle-Based Crosslinks in Polymer Networks — *S. Eileen Seo*  **1:45 Paper 81d:** Metabolomics-Guided Discovery of Metabolic Design Principles and Engineering Strategies – *Junyoung Park* 

**2:10 Paper 81e:** Hanwha Travel Award Flash Presentations

(82) Process Intensification – Novel Integration Concepts

Wednesday, Nov 8, 12:30 PM Hyatt Regency Orlando, Bayhill 28

Pranav Karanjkar, Chair Jennifer Larimer, Co-Chair

**Sponsored by:** Process Intensification & Microprocess Engineering

**12:30 Paper 82a:** Design Consideration of Multiple Dividing Wall Columns for Renewable Olefins Production Using Economic, Environmental, and Exergy Criteria – *Heehyang Kim*, *Hosanna Uwitonze, Aejin Lee, Hankwon Lim* 

12:55 Paper 82b: Improved Energy Efficiency and CO2 Emission Reduction in Dimethyl Carbonate Reactive Distillation System through Various Heat Integration Methods – *Minyong Lee*, *Heecheon Lee, Chaeyeong Seo, Jeongwoo Lee, Jae Lee* 

**1:20** Paper 82c: Ultrasonically Enhanced Chemical Processes — *Elia Colleoni*, Paolo Guida, Deoras Prabhudharwadkar, Chiara Canciani, William Roberts

#### 1:45: Break

2:10 Paper 82e: Process Intensification Based on Modular Decomposition to Improve the Sustainability of Chemical Processes — Arick Castillo Landero, Diana Dominguillo Ramirez, Aburto Jorge, Elias Martinez Hernandez

2:35 Paper 82f: Concept for the Integrated, Quasi-Continuous Production of Crystals – from the First Idea to the Industrial Pilot Plant – *Timo Dobler, Marco Gleiss, Hermann Nirschl* 

#### (83) Poster Session: Fuels and Petrochemicals Division

Wednesday, Nov 8, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

**Sponsored by:** Fuels and Petrochemicals Division

Poster 83a: Evolving Robust and Interpretable Enzymes for the Bioethanol Industry — *Anni Li, Yijie Sheng, Minghui Wang, Xiujuan Li, He Huang* 

Poster 83b: In-house Developed Resilient and Sustainable Material for Enhanced Oil Recovery - Syed Muhammad Shakil Hussain, Muhammad Shahzad Kamal, Afeez Gbadamosi, Shirish Patil, Dhafer Al-Shehri

Poster 83c: Assessing the Technical Feasibility of Steam Hydrogasification of Agriculture-Derived Wastes for Renewable Fuel Production in the Leading Agriculture Region — *Zhongzhe Liu*, *Chan Seung Park*, *Partho Roy*, *Xin Fan*, *Marco Ceja*, *Rosely Ayala*, *Robert Lozano*, *Serina Ishida* 

Poster 83d: Multiphase Particle in Cell Simulation Study of Ammonia Co-Combustion in a Circulating Fluidized Bed Combustor — Jester Lih Jie Ling, Han Saem Park, Ha Eun Lee, Seung Seok Oh, Hyun Jun Park, Sang Mun Jeong, See Hoon Lee

Poster 83e: Hydrogen Production By Oxidation of Aluminum Nanopowder in Water Under the Action of Laser Pulses – Yaroslav Kraft, Boris Aduev, Denis Nurmukhametov, Gennadiy Belokurov, Natalia Nelubina, Zinfer Ismagilov

Poster 83f: Performance Targets for Oxidative Coupling of Methane from Techno-Economic Profiling — Faisal Ashour, Mamoun Al-Rawashdeh, Patrick Linke

(84) General Poster Session

#### Wednesday, Nov 8, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

Sponsored by: Poster Sessions

Poster 84a: Machine Learning with Weighted-Soap to Efficiently Predict Electron Densities — Siddarth Achar, Leonardo Bernasconi, Karl Johnson

Poster 84b: Rapid Microfluidic Methods for Development of the Chemicals for More Efficient CO<sub>2</sub> Utilization and Sequestration – Ayrat Gizzatov, Zuhair Al Yousef, Muhammad Almajid

Poster 84c: Confined Fluid Phase Behavior of Carbon Dioxide in Nanoporous Media – Omer Salim, Keerti Sharma, Mohammad Piri

Poster 84d: Water Thin Films on Kaolinite Basal and Edge Surfaces and Their Effects on Surface Wettability in Relation to Geological Carbon Sequestration – *Minjunshi Xie, Zhehui Jin* 

Poster 84e: Revitalize Conventional Legacy OIL Fields in North Dakota with Waterflooding and CO<sub>2</sub> EOR — *Tao Jiang, Lu Jin, Stephen Guillot, Michael Warmack, James A. Sorensen, John A. Hamling, Xincheng Wan* 

Poster 84f: Development of Machine Learning [ML] Based Model for Predicting CO<sub>2</sub> Hydrate Formation Kinetics in Porous Media — Vikas Dhamu, M Fahed Qureshi, Praveen Linga

Poster 84h: A Model Selection Workflow for Assimilating Time-Lapse Seismic Data in Models for Point Bar Geologic System - Ismael Dawuda, Sanjay Srinivasan

Poster 84i: Expanding the Adsorbate Binding Energy Correlation from Pt Surface Site Stabilities to the Surface Site Stabilities of Other Metals - Shyama Charan Mandal, Frank Abild-Pedersen

Poster 84j: Predicting Surface Coverage Effects in Heterogeneous Catalysis Via an Interaction-Counting Approach – Deep Patel, Luke Roling

Poster 84k: Quantification of Self-Interaction Errors in Selective Catalytic Reduction of NOx in Zeolites — Priyanka Bholanath Shukla, Selim Romero, Rajendra Zope, Tunna Baruah, Koblar Jackson, Karl Johnson Poster 84m: An efficient and universal solar interfacial photothermal reactor toward liquid phase oxidation — *Chen Wu* 

Poster 84n: Optimization of Trickle Bed Reactor Distribution: A Computational Fluid Dynamic Approach – *Madison Holly, Carly Fox, Sebastian Uribe, Muthanna Al-Dahhan* 

Poster 840: The Design, Preparation of Metal-Organic Materials and Their Applications in Green Synthesis of API – **Yajing Shen** 

Poster 84p: Engineering Bio-MOF-1 Derived Single-Atom Catalyst with a Hierarchical Porous Nanostructure for Highly Selective CO<sub>2</sub> Electroreduction — Yechan Lee, Byoung Joon Park, Jeong Woo Han

Poster 84q: Strategies to Control the Microenvironment in Electrochemical CO<sub>2</sub> Reduction — Yaqi Cheng, Chaolong Wei, Fei Yu, Panpan Zhang, Wang Xin, **Andrew** Wong

Poster 84r: Effect of Synthesis Method on Performance of Hybrid Catalyst for Direct DME Synthesis: Flame Synthesis and Co-Precipitation. — **Onochie Okonkwo**, Komal Tripathi, Sonal Asthana, Yiming Xi, Sujit Modi, Kamal Pant, Pratim Biswas

Poster 84s: Reverse Microemulsion Synthesis Promotes the Formation of Iron Carbide in Direct Hydrogenation of CO<sub>2</sub> to Light Hydrocarbons — Yue Yu, David Simakov

**Poster 84t:** A Modeling of Flow Cell eCO<sub>2</sub>r System for Elucidating the Phenomena of Local Reaction Environment Using Multi-Physics Simulation. — *Hyeonggeon Lee*, *Ung Lee* 

Poster 84u: CO2 Upgradation By Methane Coupling on Metal Ion-Exchanged Zeolites – Sundar Raam Swaminathan, Venugopal Balashanmugam, Niket Kaisare

Poster 84v: A Structure-Guided Design of an Oligomeric Hydrophobin Bundle Using Coiled Coils — *Mohamad Mahmoud*, *Suna Jo, Won Min Park*  Poster 84w: Single Particle Cryo-EM Structure of Ferritin Biomineralization Showing the Protein-Nanoparticle Conjugate - Sagnik Sen

Poster 84x: Investigating the Potential of TMS-EDTA Modified Silica for Valuable Element Adsorption from Produced Water – Saeed Azizi, Anirban Ghosh, Songpei Xie, Mark Krzmarzick, Clint Aichele

Poster 84y: Treatment of Domestic Wastewater By Coagulation, Adsorption, and Filtration for Reusing in the Production of Concrete Mixtures — *R. Morsy, Salma O. Mahmoud, Emad El-Din E. Abdel-Qader, Kareem M. Bakr, Anas K. Taha, Ahmed M. Abdallah, Hassan M. Abdul Karim, Ahmed Mahmoud, Mohamed Mostafa* 

**Poster 84z:** High-Efficiency Solar Evaporator System for Treating Brackish and Produced Water.

— **Mounika Chevula**, Punya Mainali, Charlie Cutts, Sharad Puri, David N. McIlroy, Seokjhin Kim

Poster 84aa: Demonstration of a Batch Electrochemical System for Phosphorus Recovery from a Real Municipal Wastewater Recycle Stream — **Syed Asad Abbas**, Sana Heydarian, Lawrence Ajayi, Jason Trembly, Damilola Daramola

Poster 84ab: Enhanced Electro-Activity of Nickel Phosphide By Pre-Treatment for Efficient Hydrogen Sulfide Elimination - Xin Zhang, Riying Qi, Kuichuan Sheng, Ruo He, Hongjian Lin

Poster 84ac: Modified Donnan Dialysis Process for Selective Nutrient Removal from Agricultural Liquid Waste — *Amir Akbari, Lauren F. Greenlee, Bruce E. Logan* 

Poster 84ad: A Stochastic Optimization and Machine Learning-Based Framework for Evaluating Ammonia Utilization As a Hydrogen Carrier – **Dongjun** Lim, Jiwon Gu, Jong Ah Moon, Yeong Jin Koh, Hankwon Lim

Poster 84ae: Electrochemical Capacitance Tuning of Carbon Nanosheets Using a Salt-Template Process — **Devapriya Basu**, Ramesh Achayalingam, M. Sterlin Leo Hudson Poster 84af: Developmental Pb Exposure Increases AD Risk Via Altered Intracellular Ca<sup>2+</sup> Homeostasis in hiPSC-Derived Cortical Neurons – Junkai Xie, Shichen Wu, Chongli Yuan

Poster 84ag: Analysis of Internal Flow Phenomena in a High Speed Rotating Cylinder Using Double Parabolic Axial Flow Model – *Dr. Sahadev Pradhan* 

Poster 84ah: Soiling Impacts on Hydrophobic Coating with and Without Dew Suppression — Aniket Ratnaparkhi, Drashti Dave, Michael Valerino, Mike Bergin, Chinmay Ghoroi

Poster 84ai: Effect of Water-Gas Seepage and Salt lons on Hydrate Phase Transition in Porous Media - Huiru Sun

Poster 84aj: Persistence of *Phi6*, a Sars-Cov-2 Surrogate, in Simulated Indoor Environments: Effects of Humidity and Material Moisture Adsorption — *Eloise Parry-Nweye*, *Zhenlei Liu*, *Yousr Dhaouadi*, *Xin Guo*, *Jianshun Zhang*, *Dacheng Ren* 

Poster 84ak: Multi-Objective Optimization for Work-Integrated Heat Exchange Network — Yongjian Huang, **Yu Zhuang**, Linlin Liu, Jian Du, Shengqiang Shen

Poster 84al: Pre-Differentiation Pfas Exposure and Its Effect in Human Dopaminergic-like Neurons — **Shichen Wu**, Junkai Xie, Han Zhao, Xihui Zhao, Chongli Yuan

Poster 84am: Sustainable Detection of Oil at Well Site: High Contrast UV Fluorescence Imaging System for Pixel-Level Detection of Oil-Bearing Rock Cuttings — Richa Sharma, Karim Bondabou, Mahdi Ammar, Matthias Francois

Poster 84ao: A Novel Approach to Develop Industrial Facility's Life-Time Energy Efficient Design Zeeshan Farooq & Abdulrahman Hazazi, Energy System Division, P&csd Saudi Aramco, Dhahran – Zeeshan Faroog

Poster 84ap: Economic and Environmental Assessment of Plastic Sorting and Recycling: A Multi-Period Approach – *Cheon JaePil, Junhyeok Son, Yuchan Ahn*  Poster 84aq: Maximizing Cost Savings and Reducing CO2 Emission in NCC Process with Heat Exchanger Networks: An Integrated Analysis – **Subin Jung**, Hyojin Jung, Yuchan Ahn

Poster 84ar: Techno-Economic Assessment of Biomass to Valuable Pyrolyzed Hydrochar Via Hydrothermal Carbonization and Pyrolysis. — Cadianne Chambers, Toufiq Reza, Sumit Sharma, Nirupam Aich

Poster 84as: Application of a Developed Techno-Economic Analysis Framework to CO2 Electrochemical Reduction Processes — *Claudemi Alves Nascimento*, *Fernando V. Lima* 

Poster 84at: Asset Intensification: Application of Modelling Tools and Methodologies from a Cdmo Perspective — *Filipe Ataide, Jose Luis Santos, Filipe Gaspar* 

Poster 84au: Developing Efficient and Sustainable Packaging Processes in the Downstream Operations of the Oil and Gas Sector — **Swapana Jerpoth**, Barnabas Gao, Robert Hesketh, C. Stewart Slater, Mariano J. Savelski, Kirti Yenkie

Poster 84av: Economic Comparison of Nano-Porous Silica Production Processes from Rice Husk and Sand — *Semie Kim*, *Young-II Lim* 

Poster 84aw: Optimizing Reformer Performance for Integrated Blue Hydrogen-Methanol Production: A Multi-Objective Optimization and Techno-Economic Study – Ajay Koushik V, Achyuta Krishnan, Niket Kaisare, Preeti Aghalayam

Poster 84ax: Life Cycle Assessment of Biodiesel Production Processes from Waste Animal Fats with Pretreatment Process — **Pyeong-Gon Jung**, Semie Kim, Young-II Lim

Poster 84ay: Catalytic Performance Promotion of Pd Cluster Towards H<sub>2</sub>O<sub>2</sub> Production By Potential-Driven Coordination Adjustment – *Zhiping Deng*, *Xiaolei Wang* 

Poster 84az: Stability and Redox Kinetics of Ti<sup>4+</sup>/Ti<sup>3+</sup> for Flow Battery Applications — *Maria Bruce, Vijay Ramani*  Poster 84ba: Highly Efficient Redox Flow Batteries Using Low Cost Materials — *Abena Williams*, *Robert Emmett, Xueting Wang, Eric M. Davis, Mark E. Roberts* 

Poster 84bb: Understanding the Role of Calcium Zincate (CaZn<sub>2</sub>(OH)<sub>6</sub>·2H<sub>2</sub>O) in Improving Cycle Life of Rechargeable Alkaline Zinc Batteries – *Patrick K. Yang*, Damon E. Turney, Michael Nyce, Timothy N. Lambert, Stephen O'Brien, Sanjoy Banerjee, Gautam Yadav, Jinchao Huang, Meir Weiner, Shinju Yang

Poster 84bc: Effects of Composite Sulfur Electrode Structures and Electrolyte Compositions on Rechargeable Aluminum-Sulfur Batteries – Snehal Bhalekar, Robert Messinger

Poster 84be: Efficient Scalable Hydrothermal Synthesis of MnO<sub>2</sub> with Controlled Polymorphs and Morphologies for Enhanced Battery Cathodes – *Shifeng Hong, Shuo Jin, Lynden A. Archer* 

Poster 84bf: Imidazole-Based Concentrated Hydrogen-Bonded Electrolytes for Energy Storage Applications – *Miguel Muñoz Sánchez, Burcu Gurkan, William Dean* 

Poster 84bg: Effect of Cathode Precursor Particle Size Distribution on Cobalt-Free Lithium-Nickel-Manganese-Oxide Battery Performance – *Sunuk Kim*, Sourav Mallick, Arjun Patel, Jethrine Mugumya, Sophie Kothe, M. Parans Paranthaman, Michael L. Rasche, Ram Gupta, Herman Lopez, Mo Jiang

Poster 84bh: High-Throughput Screening of Electrosynthetic Reactions Enabled By Wireless Electrochemical Cell — *Yiming Mo* 

Poster 84bi: Increasing Data Collection Efficiency through Incorporation of Derivative and Uncertainty Information into Gaussian Process Regression – Jacob Monroe, William P. Krekelberg, Austin McDannald, Vincent K. Shen

Poster 84bj: Data-Driven Design of Selective Partial Agonist for Cannabinoid Receptors — Soumajit Dutta, Austin Weigle, Diwakar Shukla Poster 84bk: Removal of Insecticides from Wastewater Using Ionic Liquids: A Computational Study — *Mustafa Nasser*, *Mohammed Al Hassan*, *Ibnelwaleed Hussein*, *Muneer Ba-Abbad*, *Imran Khan* 

Poster 84bl: Understanding Proton-Coupled Electron Transfer on Polyoxovanadate Nanoclusters — Andreas Towarnicky, Giannis Mpourmpakis

Poster 84bm: First-Principles Mechanistic Study of Oxidative Degradation of Aqueous Amine Solvents for Carbon Dioxide Capture – *Jiwon Yu, Dipam Patel, Gyeong S. Hwang* 

Poster 84bn: A DFT Analysis of Optimal Solvents for High-Throughput Processing of Imine-Linked Covalent Organic Frameworks — *Emily Polo-Rankin, Alex Fatouros, Obioma Uche* 

Poster 244f: Investigation of Catalytic Activity of Fecunc Catalysts for Oxygen Reduction Reaction in Alkaline Medium with Gas Diffusion Electrode Half-Cell System – Jong Gyeong Kim, Hyeon-Seung Jung, Youngin Cho, Chanho Pak

#### (85) Poster Session: Process Development

Wednesday, Nov 8, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

Vinod Kumar Venkatakrishnan, Chair

**Sponsored by:** Process Development Division

Poster 85a: Internally Heat-Integrated Pressure-Swing Distillation for Non-Ideal Separation Using Computational Fluid Dynamics — Heecheon Lee, Chaeyeong Seo, Minyong Lee, Jae Lee

Poster 85b: An Energy-Efficient Double Annular Column for Azeotropic Separation — Heecheon Lee, *Minyong Lee*, Jae Lee

Poster 85d: Efficient Cleaning Methods for Gas Supply Systems in Semiconductor Manufacture Using CFD – Ireh Seo, **Rakyoung** Jeon, Tae-Ung Yoon, Chang-Ha Lee Poster 85e: Amine Blending Optimization for Maximizing CO<sub>2</sub> Absorption Capacity in a MEA -Mdea -Water System Using the Thermodynamic Model - Jinyoung CHA

Poster 85f: Techno-Economic and Environmental Assessment of Onsite Green Hydrogen Production By Ammonia Cracking — *Sijan Devkota* 

(86) Poster Session: Sustainability Science and Engineering, Biorefineries, and Energy

Wednesday, Nov 8, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

Siddharth Patwardhan, Chair Clayton Jeffryes, Co-Chair Yaseen Elkasabi, Co-Chair

**Sponsored by:** Sustainable Engineering Forum

Poster 86a: Selective and Efficient Valorization of Industrial Wastes Via Carbon Mineralization — *Ning Zhang*, *Danny Huang*, *Aaron Moment*, *Ah-Hyung Park* 

Poster 86b: Unique Synergies between Carbon Mineralization and Biomass Conversion: Alkaline Thermal Treatment for Combined Carbon Capture and Hydrogen Production – Jonah Williams, Ah-Hyung Park

Poster 86c: Evaluation of Bioenergy Production from Advanced MFC-Fermentation Technology – *Kundan Kumar*, *Ming-Hsun Cheng* 

Poster 86e: Chemical Sector Risk Management Agency Resources in Support of a Sustainable and Resilient Chemical Sector – Janine Mason, Ashley Pennington, Cheryl Louck, Jacob Mehl

Poster 86g: Landfill Gas Converted into Renewable Natural Gas: A Case Study in Texas — Helen Lou, Elizabeth Hastings, Jian Fang, Jessica Ledwith, Samantha Adelan

Poster 86h: Synthesis and Tribological Properties of Bio-Based Lubricants from Vegetable Oils — Paulo Roberto C. F. Ribeiro Filho, Francisco Murilo Tavares de Luna, Celio Cavalcante Jr. Poster 86i: Materials for Direct Air Capture of CO<sub>2</sub> Via Particle Molecular Layer Deposition - Hailey Loehde-Woolard, Bergen Evans, Kent J. Warren, Alan Weimer

Poster 86j: Integration of Sustainable Extraction and Recovery of Energy-Relevant Metals Using Aldoxime-Based Ligands Systems from Unconventional Resources — Amanda Whai Shin Ooi, Hunter B. Vibbert, Ah-Hyung Park

Poster 86k: Guidelines for Designing Amine-Based CO<sub>2</sub> Capture Systems Onboard LNG Fuelled Ships — Anikesh Kumar, Preethi Sridhar, Farooq Shamsuzzaman, Iftekhar Karimi

Poster 86m: A Novel Integration of Solar Chimney Power Plant with Wind Farm for Green Hydrogen and Distilled Water Production – Fares Almomani, Jihad Eriekat, Hamza Alnawafah, Emad Abdelsalam

Poster 86n: Electrochemical Performance of Hybrid Ferrite/(Mn, Ti)-Oxide Electrode for Asymmetric Supercapacitor — *Khang Huynh*, *Bharathkiran Maddipudi, Rajesh Shende* 

Poster 860: Data-Driven Modeling to Predict Wettability for the Rock/Hydrogen/Brine System — Shams Kalam, Muhammad Arif, Sidqi A. Abu-Khamsin, Shirish Patil, Muhammad Shahzad Kamal

Poster 243c: System Level Analysis of Intermitent Photocatalytic Processes for the Production of Liquid Fuels - Luisdomingo Guzman, Juan Manuel Restrepo-Florez

## (87) Poster Session: Transport and Energy Processes Division

Wednesday, Nov 8, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

Yangchuan Xing, Chair Zheng Chen, Co-Chair

**Sponsored by:** Transport and Energy Processes

Poster 87a: Steam Reforming of Model Biomass Gasification Tar over Ni-Based Carbon Supported Catalyst — Sang Jun Yoon, Sung Jin Park, Tae-Young Mun, Jihong Moon

Poster 87b: Effects on Ammonia Injection Directions for Coal-Ammonia Co-Firing in a Circulating Fluidized Bed Combustion Test Rig – Seong-Ju Kim, Sung Jin Park, Sang Jun Yoon, Tae-Young Mun

Poster 87c: Techno Feasibility Analysis for Steam-to-Hot Water Conversion for West Virginia University, Morgantown Campus. – Sai Kiran Yerravally, Daniel Lemasters, Thomas J. Rosson, Srinivas Palanki, Nagasree Garapati

Poster 87d: Numerical Investigations of Spontaneous Imbibition in Porous Media — Akshit Agarwal, Jyoti Phirani

Poster 87e: Stabilizing Sodium Ion Transfer at the Nasicon Solid-State Electrolyte and Metallic Na Anode Interface By Nanoscale Metal Oxide Coating — **Baiheng Li**, Ian Baker, Weiyang Li

Poster 87f: Biogas Production from Co-Digesting House Hold Vegetable Waste with the Industrial Waste Water Using Expanded Granular Sludge Bed Anaerobic Digestion (AD) System — Jackson Oglesby, Sarah Riley, Frank Reinsch, Jaden Johnson, Vena Prudent, Justin Penn, Haider Al-Rubaye, Joseph Smith

Poster 87g: Insight into Electrochemical Batch Reactor for Phosphorus Recovery Using Mathematical Modeling — Ardavan Zanganeh, Kody Wolfe, Damilola Daramola

Poster 87h: Optimization of Capacitance in Supercapacitors By Constructing an Experimentally Validated Hybrid Artificial Neural Networks-Genetic Algorithm Framework – **Betul Uralcan** 

Poster 87i: In silico Demonstration of Fast Anhydrous Proton Conduction on Graphanol - Siddarth Achar, Leonardo Bernasconi, Karl Johnson Poster 87j: Ageing Effects of Catalyst Ink for Polymer Electrolyte Membrane Fuel Cells – *Mario Kircher, Wai* Yee Koo, *Michaela Roschger, Viktor Hacker* 

Poster 87k: Electrode Development in Alkaline Direct Ethanol Fuel Cells — *Michaela Roschger*, *Sigrid Wolf*, *Boštjan Genorio, Selestina Gorgieva, Viktor Hacker* 

Poster 87I: Multi-Physics Simulations and Bayesian Optimisation of Flow in Alkaline Water Electrolyzers — *Morgan Kerhouant*, *Thomas Abadie*, *Raj Venuturumilli*, *Andre Nicolle*, *Omar Matar* 

Poster 87m: Ion and Water Transport in Polynorbornene-Based Thin Film Membranes – **Ge Sun**, Zhongyang Wang, Abhishek Sharma, Shrayesh Patel, Paul F. Nealey, Juan J. de Pablo

Poster 87n: Understanding Water Absorption, Percolation, and Ion Transport in an Anion Exchange Membrane – *Zhongyang Wang*, *Ge Sun, Mrinmay Mandal*, *Abhishek Sharma, Chuting Deng, Kai Wang, Aaron Taggart, Alex Martinson, Paul Kohl, Juan J. de Pablo, Shrayesh Patel, Paul F. Nealey* 

Poster 870: Development of High-Power and Durable MEA for Polymer Electrolyte Membrane Fuel Cells Using Structured Carbon Nanofiber Matrix – Yunseong Ji, Dae Woo Kim,

Yunggun Shul

Poster 87p: Computational High-Throughput Study of Hydrogen Permeation through Two-Dimensional Structures for Use As Proton-Conducting Membranes — Yuting Li, Daniel Bahamon, Jaber Almarri, Nirpendra Singh, Marcelo Lozada-Hidalgo, Andre K. Geim, Lourdes Vega

Poster 87r: Energy Optimization By Installation of Hrsg (HEAT RECOVERY STEAM GENERATOR) at Exhaust Gases of Gas Turbine Driven Compressor — *Kashif Jameel, Usman Asif* 

#### (88) Plenary Session: Computational Molecular Science and Engineering Forum (Invited Talks)

Wednesday, Nov 8, 3:30 PM Hyatt Regency Orlando, Rock Spring I/II

Jeetain Mittal, Chair Sapna Sarupria, Co-Chair

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

**3:30** Paper 88a: Accelerating discovery with computational chemistry in challenging materials spaces – *Heather Kulik* 

**4:10 Paper 88b:** Computational and Experimental Characterization of the Ligand Environment of a Ni-Oxo Catalyst Supported in Metal–Organic Framework NU-1000 — Stephen Vicchio, Zhihengyu Chen, Karena Chapman, **Rachel Getman** 

4:30 Paper 88c: T.B.A – Rebecca Lindsey

5:10 Paper 88d: Electronic Structure and Reactivity Predictions for Soft Material Length Scales — *Nicholas Jackson* 

5:30 Paper 88e: Understanding the Effect of Water on CO<sub>2</sub> Capture in Metal-Organic Frameworks — Maytham Alzayer, Filip Formalik, Faramarz Joodaki, Srinivasu Kancharlapalli, Jiayang Liu, Randall Snurr

(89) Innovation and Entrepreneurship in Chemical Engineering

Wednesday, Nov 8, 3:30 PM Hyatt Regency Orlando, Bayhill 17

Saurabh Maduskar, Chair Udit Gupta, Co-Chair Nitish Mittal, Co-Chair

**Sponsored by:** Management Division

3:30: Welcoming Remarks

**3:40 Paper 89d:** Fueling the Energy Transition – Lessons Learned from a Renewable Energy Startup – *Derek Vardon*  4:05 Paper 89e: Scale-up of Purecycle Purification Process — *Michael Weber* 

**4:30** Paper 89a: Trials and Tribulations in Entrepreneurship for a Chemical Engineer – *Andrew Jones* 

4:55 Paper 89b: Gambling on Innovation with Learning — *Darrell* Velegol

**5:20 Paper 89c:** Our Journey in Commercialising Scalable, Economical and Sustainable Porous-Silicon for Li-Ion Battery Anodes — *Siddharth Patwardhan* 

5:45: Concluding Remarks

(90) Division Plenary: North American Mixing Forum Awards Session (Invited Talks) Wednesday, Nov 8, 3:30 PM Hyatt Regency Orlando, Bayhill

Hyatt Regency Orlando, Bayhill 31

Sujit Bhattacharya, Chair David Dickey, Co-Chair Richard Cope, Co-Chair

**Sponsored by:** North American Mixing Forum

3:30 Paper 90a: Student Award Presentation – *Sujit Bhattacharya* 

3:45 Paper 90b: "Process Always Comes First" When Successfully Applying Mixing Technology - Aaron Sarafinas

(91) Fundamentals and Applications for Municipal Solid Waste Treatment and Valorization

Thursday, Nov 9, 8:00 AM Hyatt Regency Orlando, Rainbow Spring I/II

Matthew Alexander, Chair Enoch Nagelli, Co-Chair Mohamed Mostafa, Co-Chair Robert Peters, Co-Chair Aurora del Carmen Munguía-López, Co-Chair

**Sponsored by:** Solid and Hazardous Waste

8:00 Paper 91a: Integration of the Carboxylate Platform with Mcl-PHA Fermentation to Enable a Universal Route from Waste to Bioplastics — Jorge Arreola Vargas, Bing Xu, Zach Foudeh, Cheng Hu, Cesar Granda, Susie Dai, Shuhua Yuan

8:20 Paper 91b: Technoeconomic Assessment of Emerging Technologies for the Enhancement of Anaerobic Digestion Processes at Municipal Wastewater Treatment Facilities – Peter Valdez, Lesley J. Snowden-Swan, Timothy E. Seiple, Phillip Teller, Richard Garrison, Fuad Ale Enriquez, Nalok Dutta, Anthony Giduthuri, Birgitte Ahring

8:40 Paper 91c: Hydrothermal Liquefaction of Waste Activated Sludge: Initial Composition Effects on Product Distribution and Nutrient Recovery – João Poli, Susan Williams, Belinda S.M. Sturm

9:00 Paper 91d: Tracking Nitrogen Fate in US Wastewater Treatment Plants: A Case Study of Metropolitan Water Reclamation District of Greater Chicago (MWRD) Plants – Justin Chang

9:20 Paper 91e: Process Modeling, Techno-Economic Analysis and Life-Cycle Assessment of Intensified Biogas to Liquid (IBGTL) Process. — Rarosue Amaraibi, John Kuhn, Babu Joseph

9:40 Paper 91f: Elucidation of Change in Oxidation State for Metal Recovery from WTE Ash in Reactive Environments – Janhvi Trivedi, Marco J. Castaldi

10:00 Paper 91g: On-Site Electricity Generation Using Trashology's Pur-Gen Technology – William Wang, Matthew Young, Stephen Armstrong

10:20 Paper 91h: Recovery of Resources from Food Waste to Synthesise Nutrient-Loaded Slow-Release Hydrogel – Yen Wah Tong

# (92) Crystallization in Process Development

Thursday, Nov 9, 8:00 AM Hyatt Regency Orlando, Bayhill 19

Thomas Vetter, Chair Bruce Hook, Co-Chair

**Sponsored by:** Solids Flow, Handling and Processing

8:00 Paper 92a: Development of Automated Milling Platform for Crystal Engineering — Shailesh Agrawal, Saurin Hiren Rawal, Jeremy Merritt

8:25 Paper 92b: Process Control and Design of the Continuous Crystallization of a Polymorphic Agrochemical – *Montgomery Smith*, Paul Larsen, Venkateswarlu Bhamidi, Zoltan Nagy

8:50 Paper 92c: Recovery of Valuable Metals from Industrial Leachates of Spent Ni Metal Hydride Batteries By Precipitation Processes. — *Boris Guzhov, Laurent Cassayre, Nicolas Coppey, Béatrice Biscans* 

9:15 Paper 92d: Stabilization and Coagulation of Colloidal Suspensions during Crystallization - Xiongtao Ji, Ting Wang, Na Wang, Xin Huang, Hongxun Hao

(94) Fundamentals and Applications for Waste Treatment and Valorization I

Thursday, Nov 9, 12:30 PM Hyatt Regency Orlando, Rainbow Spring I/II

Heriberto Cabezas, Co-Chair Yinlun Huang, Co-Chair Robert Peters, Co-Chair Aurora del Carmen Munguía-López, Co-Chair

Sponsored by: Fundamentals

**12:30 Paper 94a:** Lessons Learned: Case Histories of Several Environmental Disasters and Their Implications for the Waste Plastics Crisis — *Jeffrey Seay, Mary Ellen Ternes, Robert Peters* 

**12:48 Paper 94b:** Methods for Al-Enabled Water Treatment — *Da Yan, Robert Peters, Yang Zhou, Mohamed Mostafa*  **1:06** Paper 94c: Valorization of Water Treatment Plant Residuals to Biodegradable Deicers — *Alexander Mathews* 

**1:24 Paper 94d:** Bio-Electrochemical Treatment of Dairy Manure for in-Situ Sulfide Remediation — *Lingkan Ding, Bo Hu* 

**1:42 Paper 94e:** A Novel Three-Stage Process to Treat Sewage Sludge with High Phosphorus Recovery and Bioenergy Production – *Lingkan Ding, Daniel Jurado Pineda, JAMES Postiglione, Bo Hu* 

2:00 Paper 94f: A Systematic Study of Co-Digestion of Fishery Sludge and Food Waste for Biogas Production — *Reza Khorasani*, *Jin Wang, Q. Peter He* 

2:18 Paper 94g: One-Pot Synthesis of a Novel Chitosan-Based Hydrogel By C-Mannich Reaction and Screening of Its Cu (II) Uptake — John Rey Romal, Dr. Say Kee Ong

(95) Advances in machine learning and intelligent systems I

Sunday, Nov 5, 3:30 PM Hyatt Regency Orlando, Bayhill 23

Mingjian Wen, Chair Wentao Tang, Co-Chair

**Sponsored by:** Information Management and Intelligent Systems

**3:30 Paper 95a:** A Novel Approach for VOC Emission Characteristics Identification Based on Deep Learning and Its Application in Source Tracing of a Chemical Industrial Park – *Deji Jing* 

**3:51 Paper 95b:** Bayesian Optimization for Nonlinear Model and Force Field Calibration — *Montana Carlozo*, Bridgette Befort, Ning Wang, Edward Maginn, Alexander Dowling

**4:12** Paper 95c: Al-Driven Hypergraph Network of Organic Chemistry: Applications in Reaction Classification – *Vipul Mann, Venkat Venkatasubramanian* 

**4:33 Paper 95d:** Machine Learning Full Elastic Tensors of Inorganic Materials with Equivariant Neural Networks — *Mingjian Wen*  **4:54 Paper 95e:** Automated Mechanism-Based Explanation Generation of Machine Learning Models – *Arijit Chakraborty, Venkat Venkatasubramanian* 

5:15 Paper 95f: Automating the Search for New Drugs: From Prediction to Characterization and Back Again — *Matthew A. McDonald*, Brent Koscher, Richard Canty, Frank Lee, Klavs Jensen

5:36 Paper 95g: A Compressed Sensing Framework for Learning Interpretable Molecular Property Models from Limited Data: Application to Discovery of Sustainable Battery Materials - Farshud Sorourifar, Madhav Muthyala, Joel Paulson

(96) Highly Efficient DOE for Rapid Process Development

Sunday, Nov 5, 3:30 PM Hyatt Regency Orlando, Celebration 6

Mark Anderson, Chair

Sponsored by: Miscellaneous

**3:30 Paper 96a:** Highly Efficient DOE for Rapid Process Development — *Mark Anderson* 

(97) Fluid Particle Separations in Energy and Environmental Systems

Sunday, Nov 5, 3:30 PM Hyatt Regency Orlando, Coral Spring I/II

Jenifer Gomez Pastora, Chair Seyi Odueyungbo, Co-Chair

**Sponsored by:** Fluid-Particle Separations

**3:30** Paper 97a: Recycling of Lithium-Ion Batteries: Selective Leaching of Lithium By Using Water As Sustainable Leaching Agent – **Rafaela Greil**, Joevy Chai, Georg Rudelstorfer, Susanne Lux

**3:55 Paper 97b:** Acoustic Oil-Water-Fines Separation for Sustainable Oil Production Operations — *Amr Abdel-Fattah*  **4:20** Paper 97c: Elucidating the Mechanisms of Ion Permeation through Sub-Nanometer Graphene Pores: Uncovering Free Energy Barriers Via High-Throughput Molecular Simulations" – *Andres Ordorica, Piran Kidambi, Peter T. Cummings* 

# (98) CO<sub>2</sub> Capture for Industrial Point Sources

Sunday, Nov 5, 3:30 PM Hyatt Regency Orlando, Regency Ballroom T

David Hopkinson, Chair Jonathan Stickel, Co-Chair Tae Hoon Lee, Co-Chair

Sponsored by: Sustainable Energy

**3:30 Paper 98a:** Increasing Diffusion Selectivity Via Free Volume Manipulation (FVM) and *in Situ* Thermal Oxidative Crosslinks of Amine-Functionalized PIM-1 Membrane — **Taigyu Joo**, Tae Hoon Lee, Wan-Ni Wu, Sungsool Wi, Zachary P. Smith

**3:48 Paper 98b:** Selective CO<sub>2</sub> Separation By Facilitated Transport in Ionic Liquid Gel Membranes — *Philip Cox, Alex Ferguson, Vincent Storhaug* 

**4:06** Paper 98c: CFD Modeling of Flue Gas Separation with Hollow Fiber Modules and Experimental Verification Via 3D Printing — Victor A. Kusuma, Lili Sun, Comfort Oluleke, Lingxiang Zhu, Nathan Diemler, Grigorios Panagakos, Glenn Lipscomb, David Hopkinson

4:24 Paper 98d: CFD Modeling of High-Flux Plate-and-Frame Membrane Modules for Post-Combustion Carbon Capture – Cheick Dosso, Lingxiang Zhu, Victor A. Kusuma, David Hopkinson, Lorenz Biegler, Grigorios Panagakos

**4:42** Paper 98e: Development and Evaluation of Novel Biphasic Solvents for Post-Combustion Carbon Capture — **Yongqi Lu**, Hong Lu, Hafiz Salih, Paul Nielsen, Qing Ye 5:00 Paper 98f: Data-Driven Design and Characterization of Aprotic *N*-Heterocyclic Anion (AHA) Ionic Liquids for CO<sub>2</sub> Capture – *Austin N. Keller*, *Pranav J. Thacker, Louise M. Cañada, Michael Baldea, Mark* 

Stadtherr, Joan Brennecke **5:18 Paper 98g:** Simulation and Uncertainty Quantification of a Cryogenic Carbon Capture System for Cement Industry — Brandon Paul, Daison Manuel Yancy Caballero, Miguel A. Zamarripa, Benjamin P. Omell, Michael S. Matuszewski

**5:36 Paper 98h:** Continuous Carbon Capture Via Oxygen/Water Electrolysis in a Modular Solidelectrolyte Reactor — *Peng Zhu, T Alan Hatton, Haotian Wang* 

(99) Division Plenary: CAST (Invited Talks)

Monday, Nov 6, 8:00 AM Hyatt Regency Orlando, Regency Ballroom Q

Carl Laird, Chair Matt Bassett, Co-Chair

**Sponsored by:** Computing Systems and Technology Division

8:00 Paper 99a: CAST Division Update — *Matt Bassett* 

8:10 Paper 99b: CAST Division Programming Update – Carl Laird

8:20 Paper 99c: Autocompletion of Piping and Instrumentation Diagrams (P&IDs) with Artificial Intelligence – Artur M. Schweidtmann

8:45 Paper 99d: Case Studies on the Combined Identification and Offset-Free Control of Chemical Processes — *Steven Kuntz*, *James J. Downs, Stephen M. Miller, James Rawlings* 

**9:10 Paper 99e:** Decision-Focused Surrogate Modeling for Mixed-Integer Optimization — *Shivi Dixit*, *Rishabh Gupta, Qi Zhang*  9:35 Paper 99f: Strategies for Renewable Muconic Acid Production from Lignin-Based Aromatics through Rational Metabolic Engineering of *Pseudomonas Putida KT2440* — Antonis Kokossis, Pinelopi Marina Politi, Stefanos Xenios, Konstantinos Mexis, Vassily Hatzimanikatis, Ljubisa Miskovic, Ilias Toumpe

**10:00 Paper 99g:** Measure This, Not That: Pareto Optimal Trade-Offs between Model-Based Information Content and Measurements Cost – *Jialu Wang*, *Alexander Dowling* 

(100) 3D Culture: Organoids and Spheroids

Monday, Nov 6, 8:00 AM Hyatt Regency Orlando, Celebration 3

Molly Kozminsky, Chair Quinton Smith, Co-Chair Sasha Cai Lesher-Pérez, Co-Chair

**Sponsored by:** Engineering Fundamentals in Life Science

8:00: Break

8:18 Paper 100a: Evaluating the Impact of Dynamic Flow on the Chemotherapeutic Treatment of Advanced Multicellular Pancreatic Cancer Models — *Priyanka Gupta, Hemant Kocher, Bhumika Singh, John Malcolm Wilkinson, Pedro Perez-Mancera, Eirini Velliou* 

8:36 Paper 100b: Development of a High-Throughput Drug Screening Platform Via Pipetting Gel Droplet Micro-Organoids Models – Daniel Montes, Fei Fan, Liao Chen, Xin Lu, Sharon Stack, Donny Hanjaya-Putra, Hsueh-Chia Chang

8:54 Paper 100c: Investigating the Role of Metabolism in Human Stem Cell Differentiation and Development Using Organoid Models – *Gautami Kelkar, Albert J. Keung* 

9:12 Paper 100d: A Human iPSC-Derived Brain-on-Chip to Model Delivery to the Brain – *Rebecca L. Pinals, Alice Stanton, Nhat Truong, Claudia F. Lozano Cruz, Adele Bubnys, Emre Agbas, Sydney Hawkins, Alexandra Volkova, Dong Shin Park, Alan Jiang, Colin Staab, Robert Langer, Li-Huei Tsai*  **9:30 Paper 100e:** Glioblastoma Organoids Model Extracellular Matrix Heterogeneity — *Alexandra Avera*, *Taylor Schnorbus*, *Macy Birge*, *Yonghyun* (John) Kim

**9:48 Paper 100f:** Invited Talk: Engineered Systems for Studying Lung Injury and Disease — *April Kloxin* 

(101) Process Intensification and Modular Manufacturing: Modeling and Simulation

Wednesday, Nov 8, 8:00 AM Hyatt Regency Orlando, Celebration 16

Ignasi Palou Rivera, Chair Fadhil Al-Aboosi, Co-Chair

Sponsored by: Process Intensification & Modular Chemical Processing

8:00 Paper 101a: Modeling and Optimization of Upfront Nitrogen Removal from LNG Baseload Plant Using Lithium Cycle – Fares Almomani, Abdullah Omar 8:20 Paper 101b: Thermodynamic Modeling of CO<sub>2</sub> Absorption in K<sub>2</sub>CO<sub>3</sub>-H<sub>2</sub>o Solution with Association Enrtl Model — *Cheng-Ju Hsieh*, *Viraj Patil, Chau-Chyun Chen* 

8:40 Paper 101c: Optimal Operation of Intensified Fluidized Bed Membrane Reactor for Oxidative Coupling of Methane - Moustafa Ali, Dustin Kenefake, Yuhe Tian, Efstratios Pistikopoulos

9:00 Paper 101d: Techno-Economic Optimization of Heat-Integrated Multi-Functional System of Catalytic Reactors: The Case of Water-Gas Shift and COS Hydrolysis Reactions — **Pranav Kherdekar**, Shantanu Roy, Divesh Bhatia

**9:20 Paper 101e:** Machine Learning Aided Process Design and Intensification Using Sparse Experimental Data: An Ammonia Production Example — *Md Al Masud*, *Yuhe Tian* 

9:40 Paper 101f: Effect of Ethylene Oxide Reactor Intensification on the Downstream Processes — Chinmoy Basak Mukta, Selen Cremaschi, Mario Eden