

147 - Meet the Industry Candidates Poster Session: Computing And Systems Technology Division

Tuesday, November 07, 2023 1:00 PM - 3:00 PM

Regency Ballroom R/S, Hyatt Regency Orlando

BOARD NUMBER	Title	First Name	Last Name	Paper Number
41	Influence of Mass Transfer for the Transient Response of Ultra-Microelectrodes to Potential and Current Transients	Cynthia	Ezeh	147a
42	Molecular Models to Predict the Influence of Templating Molecules on the Structure and Organization of Zeolites	Xuyao	Gao	147c
43	Accelerating Digitalization Via Advanced Optimization, Machine Learning, and Simulation Techniques	Pengfei	Cheng	147d
44	Machine Learning Scientist, Especially for Chemicals, Materials, Multi-Omics, Health, and Environment.	Prateek	Verma	147e
45	Quantifying Synergy for Mixtures of End-Scission and Random Scission Catalysts in Polymer Upcycling	Ziqiu	Chen	147f
46	Development of Algorithms for Identification of Sparse Dynamic Models with Mass and Energy Conservation from Noisy Data	Samuel	Adeyemo	147g
47	Reimagining Catalyst Reactivity Prediction with Machine Learning: From Data to Software Development	Xue	Zong	147h
49	Advances in Next Generation Cyber-Physical Systems: Cybersecurity, Quantum Computing, and Smart Material Design	Keshav	Kasturi Rangan	147i
50	Bridging Thermal and Electrochemical Catalysis: Rational Catalyst Design at Atomic Scales through Physical and Machine-Learning Based Insights	Shyam	Deo	147j
51	Machine Learning-Based Prediction of Thermal Conductivity in Metal-Organic Frameworks	Meiirbek	Islamov	147k
52	Modeling Kerogen Flexibility upon Gas Adsorption Using Osmotic Ensemble Simulations	Shivam	Parashar	147l
53	Control Advances for Dynamic Cyber-Physical Systems Incorporating Structural Simulation Methods and Quantum Computation	Kip	Nieman	147m
54	Hybrid Grey-Box Modeling and Estimation for Condition Monitoring of Complex Dynamics Energy Systems	Vivek	Saini	147n
55	A Novel Framework for Design of Net-Zero Chemical Systems: Analysis and Results	Amrita	Sen	147o
56	State Estimation and Cost Optimal Sensor Network Design for Electrochemical Sensor Based Corrosion Monitoring	Chandra Sekhar	Somayajula	147p
57	Optimization-Based Strategies for Decarbonization of Energy Systems	Kaiyu	Cao	147q
58	Techniques to Assist the Human-in-the-Loop in Type-1 Diabetes and Smart Manufacturing	Mrunal	Sontakke	147r
59	Data Analytics Enabled High Throughput Material Discovery and Computational Analyses for Membrane Innovations	Xinhong	Liu	147s
60	Computational Exploration of Single Atom Catalysts Supported on Metal Oxides for Sustainable Hydrogenation Reactions	Jeremy	Hu	147t
61	Optimization-Based Strategies for Spectral Analysis and Kinetic Modeling	Thomas	Krumpolc	147u
62	Enhancing Feature Engineering and Machine Learning through Systems Engineering for Improved Diagnosis: Case Studies in Speech Disorder and Autism Spectrum Disorder	Farnaz	Yousefi Zowj	147v
63	Rational Design of Low-Dimensional Catalysts Using First Principles Methods for CO ₂ Reduction to C ₁ Products	Lavie	Rekhi	147w
64	Evaluating Impacts of Carbon Taxes on the Economic Viability and Carbon Footprint of Plastic Production Pathways	Bo-Xun	Wang	147x
65	Development of Mathematical Programming Models for the Synthesis of Reactor Networks	Arthur Eduardo	Pastore De Lima	147y
66	Harnessing Molecular Simulations and Machine Learning to Predict Macromolecular Properties and Drive Efficient Polymer Recycling	Maria	Ley Flores	147z

BOARD NUMBER	Title	First Name	Last Name	Paper Number
67	Nonconvex Optimization Problems Involving the Euclidean Distance	Anatoliy	Kuznetsov	147aa
68	Tuning Strategy for a Multi-Objective Model Predictive Control for Cost and Emissions Optimization of Heat Pump Water Heaters	Loren	dela Rosa	147ab
69	Empowering Molecular Simulations with Machine Learning to Understand and Engineer Molecular Systems	Siva	Dasetty	147ac
70	Path-Sampling and Machine Learning for Rare Un-postulated Abnormal Events	Vikram	Sudarshan	147ad
71	Data-Driven Process Monitoring and Control for Smart Manufacturing	Lucky	Yerimah	147ae
72	Molecular Modeling and Machine Learning-Based Design and Discovery of Nanoporous Material for Energy and Environmental Applications	Krishnendu	Mukherjee	147af
73	Analysis and Optimal Design of Membrane Processes for Flue Gas CO ₂ Capture	Qinghua	Li	147ag
74	Machine Learning Enabled Development of Accurate Force Fields for Refrigerants	Ning	Wang	147ah
75	Measure This, Not That: Pareto Optimal Trade-Offs between Model-Based Information Content and Measurements Budget	Jialu	Wang	147ai
76	Effective Control of High Temperature Steam Electrolyzer Modules That Use Variable, Renewable Electricity	Jake	Immonen	147aj
77	Understanding Chromatographic Retention and Fluid Phase/Sorption Equilibria By Molecular Simulations and Thermodynamic Modeling	Chun-Kai	Chang	147ak
78	Simulation, Optimization, and Machine Learning Methods for Sustainable Process and Supply Chain Design	Yuqing	Luo	147am

223 - Meet the Industry Candidates Poster Session: Nuclear Engineering Division

Tuesday, November 07, 2023 1:00 PM - 3:00 PM

Regency Ballroom R/S, Hyatt Regency Orlando

BOARD NUMBER	Title	First Name	Last Name	Paper Number
79	Understanding the Effects of Gamma Radiation on the Chemical and Physical Characteristics of Potential Coolants for Organic Cooled Reactors	Angel	Vasquez	223a
80	Low-Cost and Highly Efficient Materials for Grid-Scale Renewable Energy Storage Devices	Abena	Williams	223b

287 - Meet the Industry Candidates Poster Session: Particle Technology Forum, North American Mixing Forum, and

Tuesday, November 07, 2023 1:00 PM - 3:00 PM

Regency Ballroom R/S, Hyatt Regency Orlando

BOARD NUMBER	Title	First Name	Last Name	Paper Number
81	Synthesis of Bio-Based Porous Materials and Their Applications	Mairui	Zhang	287a
82	Rheo-Electric Analysis of Carbon Black Suspensions Undergoing Shear-Induced Microstructural Rearrangement	Paolo	Ramos	287b
83	Stress Development in Drying Aqueous Particulate Coatings	Annie	Moorhead	287c
84	Biomaterials of Tomorrow: The Rheology of Liquefied Feedstocks and the Impact of Feedstock Variability	Diana	Ramirez Gutierrez	287d
85	Utilization of Industrial Waste, Biomass and Its Derivatives in 3D Printing Applications	Anqi	Ji	287e
86	Develop Novel Polymer Sorbents Via Combining 3D Printing and Phase Separation Techniques	Jialing	Xu	287f
87	Plastic Wastes Gasification: Versatile Metal Oxide Redox Gasification Pathways for Conversion of Post-Consumer Waste Plastics into Energy Carriers	Rushikesh	Joshi	287g
88	Advancing Granular Mixing Techniques: Unraveling the Influence of Particle Shape and Segregation in Solid-Solid and Gas-Solid Systems	Sunil	Kumar	287h
89	Pathways to Make the Precious Platinum Metals Even More Valuable	Honghong	Shi	287i
90	Synergy of Nanomaterials and Deep Learning for Advancing Material Science	Anastasia	Visheratina	287j
91	Surfactant-Modified Anionic Silica Nanoparticles (SANPs) for Rare Earth Element (REE) Separation Via Froth Flotation	Yuxuan	Dai	287k
92	Particle-Based Biomolecule Detection Systems for Advancements in Assay Workflows and Signal Transduction	Cooper P.	Thome	287n

# 337 - Meet the Industry Candidates Poster Session: Process & Product Development and Manufacturing in Chemicals &				
Tuesday, November 07, 2023 1:00 PM - 3:00 PM				
Regency Ballroom R/S, Hyatt Regency Orlando				
BOARD NUMBER	Title	First Name	Last Name	Paper Number
93	Computational Study of Reaction Mechanisms in Epoxide Ring-Opening Reactions By Aryl Borane Catalysts	Guanhua	Wang	337a
94	Engineering Nonequilibrium Interactions between Multi-Scale Colloids for Dynamical Control of Suspension Structure and Rheology	Yixin	Xu	337b
95	3D Printed MOF Monoliths for Sub-Ambient Direct Air CO ₂ Capture	Yuxiang	Wang	337c
96	Hybrid Modelling Approaches in Real-Time Pharmaceutical Process Management.	Rexonni	Lagare	337e
97	Bioprocess Development for Antimicrobial Production in <i>Pseudomonas Protegens</i> Emm-1	Antonino	Baez	337f
98	Indirect Hydrogenolysis of Polyethylene By Sub-Critical Butanol	Abdullah	AL Harthy	337g
99	Developing a CRISPR Base Editor for Multiplex Directed Evolution in <i>Saccharomyces Cerevisiae</i> .	Andrew	Cazier	337h
100	Characterization of Physical Aging Behavior of Polymer Brushes for Thin Film Applications	Sneha	Srinivasan	337i
101	Maturing iPSC-Derived Hepatocytes in a Multicellular Liver Organoid for Applications in Pharmacology and Toxicology	Neeti	Gandhi	337j
102	Carbon Capture and Aerosol Technology for CO ₂ Utilization	Onochie	Okonkwo	337k
103	Advancing Organic Photovoltaic Performance through Tight-Binding Modeling of Exciton and Frontier Orbitals in Conjugated Molecules and Polymers.	Vishal	Jindal	337l
104	Clarifying the Stability and Reactivity of Metal-Organic Frameworks Constructed from Zirconium and Iron in Aqueous Pollutant Degradation	Samuel C.	Moore	337m
105	Beyond Butler Volmer Equation for CO ₂ Electro-Reduction on Copper Gas Diffusion Electrodes (GDEs).	Peace	Adesina	337n
106	Exploring the Frontiers of Biotherapeutic Production and Biocatalysis	Priyanka	Nain	337p
107	Low-Field Nuclear Magnetic Resonance Signals and Applications in Unconventional Formations.	Yunke	Liu	337q
108	Microwave-Assisted Depolymerization and Upcycling of Plastic Waste to High-Value Products	Esun	Selvam	337r
109	From Waste to Value: Upgrading Food Waste to High Commercial Value Chemicals	Yagya	Gupta	337s
110	Integration of Porous Materials in Environmental Catalysis: Addressing Challenges in Emission and Sustainable Processes	Poonam	Rani	337t
48	Re-Imagining Catalyst Reactivity Prediction with Machine Learning: From Data to Software Development	Xue	Zong	337u
111	Absorbents for Renewable Ammonia Separation and Storage	Chinomso	Onuoha	337v
112	Controlling Intrinsic Defects in Zeolite Catalysts and Their Impact on Methanol to Hydrocarbons	Kumari	Shilpa	337w
113	Fundamental Understanding of Atmospheric Pressure Plasma-Catalyst Interaction for Sustainable Value-Added Chemicals Production	Garam	Lee	337x
114	Kinetic Parameters of <i>Bacillus Atrophaeus</i> in Response to Vapor and Liquid Hydrogen Peroxide at Aseptic Filler Tunnel Temperatures	Manoj	Sawale	337y
115	Advanced Separation Processes; From Development of Membranes of Vanadium Redox Flow Batteries to Elucidate the Properties of Oil-Water Emulsions	Aiswarya	Mechoor	337z
116	Total Life Cycle Optimization: A Facile Remanufacturing for Restoring Performance of Spent Li Ion Cathodes	Kasim	Adewuyi	337aa
117	Immunoengineering in Diseases and Treatments	Mohammad Aminul	Islam	337ab
118	Colloidal Nanoaggregates - <i>Nanobundles of Information</i>	Sneha	Mukherjee	337ac

BOARD NUMBER	Title	First Name	Last Name	Paper Number
119	Towards Enhanced Yield of Commodity Chemicals: Acrylonitrile and Ethylene Synthesis	Zhuoran	Gan	337ad
120	Molecular Dynamics Simulation for the Rational Design of Silk-Mimetic Materials	Jeongae	Kim	337ae
121	First-Principles Investigation of Mediated Electrochemical Carbon-Hydrogen Activations for Accessing Pharmaceutical Intermediates	Mayank	Tanwar	337af
122	Sting-Pathway Inhibition to Treat Sting-Associated Inflammatory Conditions	Lucinda	Pastora	337ag
123	Controlling Intracellular Mutagenesis: A Key to Targeted Therapeutic Strategies Against Antibiotic Resistance	Sreyashi	Ghosh	337ah
124	Fabrication of Polymeric Systems for Biomaterials for Use in Consumer Goods	Keturah	Bethel	337ai
125	Unique Mechanism of Cholesterol Crystallization in Biomimetic Systems	Dipayan	Chakraborty	337aj
126	Prediction of Protein Structure to Function Properties for Therapeutic Purposes	Sumaiya	Islam	337ak
127	Molecular Dynamics Study of Penetrant Diffusion in Dense Crosslinked Poly-n-Butyl-Acrylate Networks	Tsai-Wei	Lin	337al
128	Data-Enabled Experimental Development of Polymer-Based Organic Electronics	Rahul	Venkatesh	337am
129	Stress Responsive Small Non-Coding RNA Networks in Mycobacteria revealed By Coupled Experimental and Bioinformatic Approach	Alyssa	Ekdahl	337an
130	8-Oxo-7,8-Dihydroguanosine Alters RNA Enzymatic Degradation Behavior of Polynucleotide Phosphorylase	Lucas	Miller	337ao
131	Lanthanide Binding Tag Peptides for Rare Earth Elements Selective and Environmentally Friendly Separation Processes	Luis	Ortuno Macias	337aq
132	Gas-Phase Surface Modification to Control Catalyst Structure and Yields in Methane Dehydroaromatization	Jordy	Ramos-Yataco	337ar
133	Continuous Crystallization of Monoclonal Antibodies	Dulashani Ruwanthika	Ranasinghe Weerakkodige	337as
134	Development of Simulation Techniques to Design Semiconducting Polymers with Enhanced Charge Transport	Puja	Agarwala	337at
135	Species, Pathways, and Timescales for Plasma-Driven Nitrogen Fixation over Catalytic Surfaces	Brian	Bayer	337au
136	Understanding Dynamics of Adventitious and Cultured Virus Propagation in Plate and Suspension Cell Cultures to Improve Upstream Biomanufacturing Performance	Shiny	Samuel	337av
137	Exploring the Steady Operation of a Continuous Pilot Plant for the Di-Nitration Reaction	Mrityunjay	Sharma	337aw
138	Advancing Water Electrolysis By Improving Precious Metal Utilization in Oxygen Evolution Catalysts	Jane	Edgington	337ax
139	Wastewater As a Resource: Using Photocatalysis to Treat WW and Produce Synthetic Fuel Precursors	Rohit	Pal	337ay
140	Microkinetic Analysis of Programmable Catalysts: Beyond the Basics	Sallye R.	Gathmann	337az
141	Metabolic Engineering of <i>Escherichia coli</i> for High Production of 1,5-Pentanediol Via a Cadaverine-Derived Pathway	Xuecong	Cen	337ba
142	Computational Tools for Process Design	Steven	Sachio	337bb
143	Membrane Separation for Sustainable World with Zero-Emission Goal	Lakshmeesha	Upadhyaya	337bc
144	<i>Monitoring and Control of an Integrated Crystallization-Filtration-Drying Platform for Continuous Pharmaceutical Manufacturing</i>	Inyoung	Hur	337bd
145	Towards Sustainable Energy and Materials: Carbon Capture, Utilization and Storage	Guanhe	Rim	337bf
146	Evolving <i>Yarrowia Lipolytica</i> for Waste Mannitol Utilization	Angela	Gordillo Sierra	337bg
147	Biomass Utilization for a Sustainable Decarbonization Strategy	Jimmy	Soeherman	337bh
148	Nanomaterials for Infectious Disease Treatment	Xiaojing	Ma	337bj

BOARD NUMBER	Title	First Name	Last Name	Paper Number
149	Efficient and Sustainable Manufacture of Polymeric Composites and Their Applications in Fire Safety	Yufeng	Quan	337bk
150	Development of Electrochemical Separation Processes for Value-added Molecules	Jemin	Jeon	337bl
151	Process Modeling and Optimization in Biopharmaceutical Manufacturing	Chaoying	Ding	337bm
152	Nanotoxchip: A Novel Microfluidic Chip for Nanoparticle Safety Assessment	Preyojon	Dey	337bn
153	Electrochemical Engineering of CO ₂ Capture and CO ₂ Reduction	Hao	Shen	337bo
154	A Multiscale Molecular Dynamics Study of Skin Lipids	Chloe	Frame	337bp
155	Novel Wet Adhesives Derived from <i>Vibrio Cholerae</i> Biofilm Adhesins	Xin	Huang	337bq
156	Engineering Next-Generation Crispr Systems for Improved Cancer Drug Discovery	Andrew	Kristof	337br
157	Spectroscopic Characterization and Assignments of Nifedipine Via Computational Modeling and Experiment (FTIR, Raman, and ssNMR) and Comparisons to an Amorphous Solid	Zachary	Fondren	337bs
158	Surface Functionalization of Plastics with a Simultaneously Hydrophilic/Oleophobic Coating	Yihan	Song	337bt
159	Engineering <i>Yarrowia Lipolytica</i> for the Biosynthesis of Geraniol and Nepetalactol	Ayushi	Agrawal	337bu
160	Elucidating Electrochemical Trends and Stability of Metal-Modified Transition Metal Nitrides for Hydrogen Evolution and Alcohol Oxidation	Hansen	Mou	337bv
161	Complex Fluids and Transport Phenomena in the Pharmaceutical and Process Development Industry	Angela	Yang	337bw
162	Calorimetry of Drug-Polymer Amorphous Solid Dispersions to Probe the Influence of Polymer Excipient Physical Aging	Yejoon	Seo	337bx
163	The Effects of Dietary Conditions on Tumor Growth and Cancer Cell Invasion	Molly	Brennan	337by
164	A Systems Biology Approach to Understanding Environmental Stress Responses in Human Lung Cells	Sean	Engels	337cb
165	Improving Interfacial Stability of Argyrodite Sulfide-Based Solid Electrolytes and Lithium Electrodes Via CO ₂ Treatment	Shengchiang	Yang	337cd
166	Process Intensification for Industrial Crystallizations Via Process Control and Design Strategies	Montgomery	Smith	337ce
167	Increased T-Cell Transfection By mRNA Lipid Nanoparticles for Cell Therapy Manufacturing	Alina	Kunitskaya	337cf
168	Crystal Growth Modeling and Morphology Predictions of Organic Molecular AB Crystals	Neha	Padwal	337cg
169	Computational Modeling of Interactions Occurring in the Human Body Influenced By Disease, Pharmaceuticals, and Diet	Carley V.	Cook	337ch
170	Practical Application of Surface-Active Nanoparticles	Rong	Ma	337ci
171	Understanding and Designing Sustainable Catalytic Processes: Influence of Solvation on Alkene Epoxidations within Titanium Silicates	Ohsung	Kwon	337cj
172	Controlled Protein Capture Via Continuous Precipitation for Monoclonal Antibody Manufacturing	Jacinta	Okpanum	337ck
180	Dynamics and Control of Intensified Extractive Distillation with Preconcentration: A Case Study of Separating N-Propanol-Water with Minimum-Boiling Azeotrope	Chao	Liu	337cl
180	Dynamics and Control of Intensified Extractive Distillation with Preconcentration: A Case Study of Separating N-Propanol-Water with Minimum-Boiling Azeotrope	Chengtian	Cui	337cl
173	Advancing Concepts for High-Yield Syngas-Free Methane Valorization	Andrea	Blankenship	337cm
174	Solubility Prediction and Cocrystal Screening By COSMO-RS: From Theory to Experimental Validation	Fateme	Molajafari	337cn

BOARD NUMBER	Title	First Name	Last Name	Paper Number
175	Data-Driven Design and Characterization of AHA Ionic Liquids for CO ₂ Capture	Austin N.	Keller	337cp
176	Population Balance Modelling to understand Crystallization of Adeno-Associated Virus-based Gene Therapies	Vivekananda	Bal	337co
177	Novel Chemical Looping Scheme for Selective Methanol Oxidation to Formaldehyde	Sonu	Kumar	337cq
178	Mathematical Modeling of Diabetic Kidney Disease Progression to Elucidate Lack of Efficacy of Pharmacological Agents.	Haryana Y.	Thomas	337cr
179	Waste Plastic Characterization to Support Recycling	Ravindra	Prajapati	337cs
181	Continuous Crystallization Process Design Towards Improved Purity and Solid Forms	Sunuk	Kim	337ct
182	Material and Elemental Flow Analysis in Industrial Networks of 2 US Regions and the Impact of Introducing Bioplastic Manufacturing Industries in These Regions	Apoorva	Bademi	337cu
183	Biomanufacturing of Recombinant Adeno-Associated Virus (rAAV) for Gene Therapy: Production, Purification, and Evaluations	Kai	Chen	337cv
184	'Structure- Processing- Property' Relationship of Cellulose Nanocrystals for Optical and Sensing Applications	Sadat Kamal	Amit	337cw
185	Critical Process Parameters for the Manufacture of Dalcetrapib Nanoparticle- Carrier Particle Nanocomposite Powders	Peuli	Ghosh	337cx
186	Twisted Crystalline Morphology and Its Application in Functional Materials	Yongfan	Yang	337cy
187	Characterization of Rheological Properties and Microstructure of Thioester Networks during Degradation	Shivani	Desai	287m
188	Tyrosine Crosslinking of ELP Hydrogels for Tissue Engineering Applications	Iyeswaria	Kumarandi Pillai	337cz
189	Batch-to-Continuous Transition in Specialty Chemicals Industry: Intensified Dispersants Production	Riddhesh	Patel	337da
190	<i>In situ</i> Magnetic Microrheology of Mucus on Live Cell Cultures	Margaret	Braunreuther	337db

706 - Meet the Industry Candidates Poster Session: General Topics

Tuesday, November 07, 2023 1:00 PM - 3:00 PM

Regency Ballroom R/S, Hyatt Regency Orlando

BOARD NUMBER	Title	First Name	Last Name	Paper Number
	Matrix Stiffness Regulates Proteome Profiling of Primary Hepatocytes and Extracellular Vesicles Secretion upon Alcohol Exposure and HIV Infection	Youra	Moeun	706a
	Semi-Interpenetrating Networks (s-IPN) of Polybenzimidazole-Based Membranes for High-Temperature Pre-Combustion CO ₂ Capture	Mengdi	Liu	706b
	Multicomponent VOC Adsorption Behavior on Functionalized Adsorbents	Ojuolape	Oghenetega	706c
	Amine Functionalized Hierarchical MIL-101(Cr)/SBA-15 Composites for Enhanced CO ₂ Capture	Debarati	Mukherjee	706d
	Optimizing Water Production in Atmospheric Water Harvesting Using Composite Salt Porous Material	Mengjiao	Wu	706e
	Inhibitor Discovery for TMPRSS2 and Analysis of its Backbone Hydrogen Bonds Using a Simple Descriptor	Suraj	Ugrani	706f