360 - Poster Session: Computational Molecular Science and Engineering Forum

Tuesday, November 15, 2022 3:30 PM - 5:00 PM

North Hall E, Phoenix Convention Center

BOARD NUMBER	Title	First Name	Last Name	Paper Number
1	Exploring canyons in soft and glassy energy landscapes using metadynamics	Amruthesh	Thirumalaiswamy	360a
2	The Role of Heteroatom Placement and Chain Branching on Quaternary Ammonium Salts for Phase Transfer Catalysis	Brooks	Rabideau	360c
3	Investigating the Effect of Oxidic Functional Group on Graphene Oxide-Molybdenum Disulfide Heterostructures As Anode for Sodium-Ion Battery	Wonmyung	Choi	360d
4	A Study on the Ionic Conductivity Improvement Mechanism of Halospinel Li2Sc2/3Cl4 By Variable Li and Dopant Concentration	SuSeong	Hyun	360e
5	Redox Behavior of Single Atom Catalysts for the Upgrading of Plastic Waste-Derived Species	Jeremy	Hu	360f
6	Revisiting Nanoparticle Interactions for Effective Nanofluid Modeling and Simulation	Jee-Ching	Wang	360g
7	The Molecular Simulation Design Framework (MoSDeF): New Capabilities	Co D.	Quach	360h
8	Microbubbles As Non-Invasive Targets for Blood Brain Barrier Disruption: An *in silico* investigation	Bailey	Zinger	360i
9	Deep Reinforcement Learning As a Tool to Enable Coarse Grained Vaccine Models	Daniel	Orbidan	360j
10	Toward Accurate and Transferable Coarse-Grained Peptide Models Using Data-Driven Approaches	Luc	Christians	360l
11	Predicting Quantum-Accurate DNA Electron Densities and Forces with Equivariant Neural Networks	Alex	Lee	360m
12	Elucidating Ethylene Hydrogenation on Site Isolated Intermetallic Catalysts	Angela	Nguyen	360n
13	Electron Density Prediction with Graph Neural Networks on Large Catalyst Datasets	Ethan	Sunshine	360o
14	Exceptional Stability of Gd-Doped UO_2 Against Surface Oxidation: First-Principles Study	Minjoon	Hong	360p
15	Explaining Improvements in Li-Ion Battery Performance By Atomic Layer Deposition of Alumina Using Molecular Dynamics Simulation	Julie A.	Nguyen	360q
16	Positive Unlabeled Learning of Peptide Properties	Mehrad	Ansari	360s
17	Elucidating Ligand Selectivity and Partial Agonism Towards Cannabinoid Receptors Using Machine Learning Approaches	Soumajit	Dutta	360t
18	Molecular Simulations of Protein/Ligand-Mediated Microglial Activation in Alzheimer's Disease	Emma	Lietzke	360u
19	Coarse-Grained Molecular Dynamics Simulations of ssDNA Loaded Adeno-Associated Virus	Tibo	Duran	360v
20	Design of Pore Wall Chemistry to Control Solute Transport and Selectivity	Sally	Jiao	360w
21	Studying Anhydrous Proton Transport on Graphene-Based Materials Using Deep Learning Methods	Siddarth	Achar	360x

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BOARD NUMBER	Title	First Name	Last Name	Paper Number
22	The Nuclear and Surface Electrostatic Potential As Descriptors of Chemical Interactions	Joakim	Halldin Stenlid	360y
23	Understanding DNA Hybridization through Thermodynamics and Kinetics of Abasic Oligomers	Mike	Jones	360z
24	The Chebyshev Interaction Model for Efficient Simulations (ChIMES): Machine-Learned Interatomic Models for Quantum-Accurate Reactive Simulation	Rebecca	Lindsey	360aa
25	Inverse Design of Open Nanocrystal Superlattices Using an Oscillating Pair Potential	Chase	Petix	360ab
26	Using Text-Mining and Community Knowledge to Quantify and Engineer Stability in MOFs	Aditya	Nandy	360ac
27	Electrical Double Layer Capacitance and Polarizability Modeled Using Classical Molecular Dynamics.	Bolton	Tran	360ad
28	Insights of Phenolic Compounds Extraction from an Aqueous Environment Using Natural Deep Eutectic Solvents: Quantum Chemical and Molecular Dynamics Simulation	Nikhil	Kumar	360ae
29	Investigating the Electrocatalytic Reduction of 2,4,6-Tri-Nitro-Toluene (TNT) across Late Transition Metal Surfaces Using Density Functional Theory Methods	Andrew	Wong	360af
30	Identification of Potential TMPRSS2 Inhibitors By Virtual Screening Using Molecular Docking and Machine Learning	Suraj	Ugrani	360ag
31	Self-Assembly of Lobed Colloidal Particles into Porous Morphologies	Brunno	C. Rocha	360ah
32	Simulation of Lipid Membranes Using Coarse-Grained Model and Reverse-Mapping	Hiroya	Nitta	360ai
33	Determination of Electronic Driving Factor for Selective Adsorption of Arsenic over Phosphorous Oxoanions By Fe(III)-Crosslinked Chitosan Using DFT	Obinna	Nwokonkwo	360aj
34	Insights into the Phase Diagram of Pluronic L64 Using Coarse-Grained Molecular Dynamics Simulations	Mangesh	Bhendale	360ak
35	Understanding the Calcium-Binding Ability of Polystyrene Sulfonate in the Presence of Dodecyl Sulfate By Using Molecular Dynamics Simulations	Sonali	Gore	360am
36	Development and Validation of Non-Bonded Interaction Parameters between Coarse-Grained Amino Acid Models and Water	Esmat	Mohammadi	360an
37	Elucidating the Bulk and Interfacial Structure of Ionic Liquids from the Dilute to Concentrated Regimes Using Molecular Dynamic Simulations	Lisa	Je	360ao
38	Developing Deep Learning Models to Predict Sigma Profiles of Lignin-Derived Organic Molecules	Usman	Abbas	360ap
39	Effect of Solvent Quality on Structure and Dynamics of Lignin in Solution	Nusrat	Jahan	360aq
40	Identifying the Stoichiometry of the Metastable Cu^{3+} State in Alkaline Electrochemical Systems Using DFT-Based Theoretical Raman Standards	Lars	Ostervold	360ar

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BOARD NUMBER	Title	First Name	Last Name	Paper Number
41	Bayesian Forcefield Driven Monte Carlo and Molecular Dynamics Simulations of O and Cl Promoted Silver Surface Reconstructions	Anna	Sviripa	360as
42	Explosive Mechanochemistry: Foundations for Strength-Aware Chemical Kinetics	Matthew	Kroonblawd	360at
43	Protein Interactions Determined from Computational Methods	Gregory	Dignon	360au
44	A Computational Study for Predicting Stability Differences in Multiple Conformations of the Sars-Cov-2 Frameshifting RNA Element	Karim	Malekzadeh	360av
45	Comparison of Advanced Sampling Techniques for Atomistic Scale RNA Folding	Kosar	Rahimi	360aw
46	Understanding the Normal Bicontinuous Cubic Phase in Gemini Lyotropic Liquid Crystals in Order to Design Selective Separations	Nathanael	Schwindt	360ax
47	Parameterization of C, Si, and Ge in the Common Harmonic Form for Molecular Dynamics Simulations	Katarina	Odak	360ay
48	The Role of Antiretroviral Therapeutics As Both Inhibitors and Substrates of P-Glycoprotein	Daisy	Fuchs	360az
49	Modeling of Photoresist Pattern Formation in EUV Lithography Through Molecular Dynamics Simulations	Seungtae	Kim	360ba
50	Benchmarking Martini 3.0 Force Field for Reproducing Thermodynamic Properties of Biomolecular Condensates	Ayush	Gupta	360bb
51	Understanding Protein Unfolding Under Different Stressors from Molecular Dynamics Simulations	Yinhao	Jia	360bc
52	CCR5-Eriously? Reexamining HIV-1 Tropism Switching with *In Silico* directed Evolution	Jonathan	Faris	360bd
53	Monte Carlo Simulations Predicting Adsorption of 1,4-Dioxane in All-Silica Zeolites	Samiha	Sharlin	360be
54	Coarse-Grained Models of Polyetherketoneketone (PEKK) Used to Perform Fusion Weld Simulations and Predict Resulting Mechanical Properties.	Chris	Jones	360bf
55	Investigating Stable and Active Catalysts for Hydrogen Generation Via Methane Pyrolysis in Molten Media, Using *Ab Initio* Molecular Dynamics	Ojus	Mohan	360bg
56	Extending the MolMod Database to Transferable Force Fields	Sebastian	Schmitt	360bh
57	Mass Transfer through Vapor-Liquid Interfaces of Binary Mixtures studied by Non-Stationary Molecular Dynamics Simulations	Dominik	Schaefer	360bi
58	Theoretical Investigation of The Coverage Effect on Ni-In Intermetallic Catalysts for Selective Hydrogenation of Acetylene to Ethylene	Zahra	Almisbaa	360bj
59	Optiboost: A Method for Choosing a Safe and Efficient Boost for the Bond-Boost Method in Accelerated Molecular Dynamics (AMD) Simulations with Hyperdynamics (HD)	Jianming	Cui	360k

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#361 - Interactive Session: Applied Mathematics and Numerical Analysis

Tuesday, November 15, 2022 3:30 PM - 5:00 PM

North Hall E, Phoenix Convention Center

BOARD NUMBER	Title	First Name	Last Name	Paper Number
63	Towards Field Wide Integrated Field Asset Modelling and Associated Optimization Methods	Shakeel	Ramjanee	361a
64	Towards an Integrated Field Wide Production Optimization Approach	Shakeel	Ramjanee	361b
65	Optimal Placement of Portable and Fixed Charging Stations for Electric Vehicles Charging	Resmi	Suresh	361d
65	Optimal Placement of Portable and Fixed Charging Stations for Electric Vehicles Charging	Ayush	Bansal	361d
66	Mathematical Programming Formulations for the Optimal Generation and Transmission of Electricity in a Macroscopic System Using the Concept of Energy Hub	Vicente	Rico-Ramirez	361c
67	Neural-Network Incorporated CFD Models for Adsorption Simulation on Complex Material	Zhu	Ming	361e
68	Mathematical Modeling of Drug Release from Bi-Layered Polymer Capsules in the Eye	Eduardo A.	Chacin Ruiz	361f
69	Differentiating between FSH and HMG Dosage for Personalized Modeling of Superovulation in IVF Patients	Bhavi	Barnwal	361g
70	The Effect of Subdiffusion on the Stability of Autocatalytic Systems	Uttam	Kumar	361i
71	Extracting Thermodynamic and Fluorescent Properties of Intercalating Dyes from Temperature-Programmed PCR Measurements with Modeling and Optimization	Robert	DeJaco	361j
72	Prototype Development to Guide the Systemic Description of Biotechnological Processes	Priscila	Marques Da Paz	361k
73	Predict Transport and Deposition of Multicomponent E-Cigarette Aerosols in a Subject-Specific Airway Model with Different Nicotine Forms: An *in silico* Study	Yu	Feng	361l
74	A Robust, Multi-Model Model Predictive Control Approach to Vagal Nerve Stimulation of the Human Cardiac System.	Oluwasanmi	Adeodu	361m
75	Limits of Entrainment of Circadian Neuronal Networks	Georgios	Psarellis	361n
76	Modeling and Control of Antibody Purification Via Protein a Affinity Chromatography	Fred	Ghanem	361o
77	Influence of the Spatial Organization of Contaminants on Bioremediation	Jenna	Ott	361p
78	Energy optimization of chemical process : Comparison of derivative-free algorithms	Minsu	Kim	361q

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BOARD NUMBER	Title	First Name	Last Name	Paper Number
	# 362 - Interactive Session: Data and Information Systems			
	Tuesday, November 15, 2022 3:30 PM - 5:00 PM			
	North Hall E, Phoenix Convention Center			
81	A Reinforcement Learning Approach for Stochastic Cutting Stock Problem	Jie-Ying	Su	362a
82	Multi-objective Optimization of Process Efficiency and CO2 Emission for On-Site Hydrogen Production Process Using Hybrid Data-Driven Model.	Jaewon	Lee	362b
83	Data-Driven Surrogates with Physics-Informed Architecture for Modelling Non-Linear Stiff Dynamic Systems	Suryateja	Ravutla	362c
84	A Comparative Evaluation of Machine Learning Algorithms in Predicting Syngas Fermentation Outcomes Using Limited Experimental Data	Garrett W.	Roell	362e
85	Development of Bayesian Machine Learning Algorithms for Optimal Nonlinear Model Selection and Parameter Estimation from Noisy Data of Unknown Characteristics	Samuel	Adeyemo	362f
86	Soft Actor-Critic Deep Reinforcement Learning with Hybrid Actions for Scheduling of Energy Systems Under Demand Response	Gustavo	Campos	362g
87	Physics Informed Machine Learning for Feasibility Analysis	Zachary	Kilwein	362h
88	Virtual Sample Generation Based on Quantile Regression Variational Generative Adversarial Network for Soft-Sensing Modeling	Xunyuan	Yin	362i
89	Rnn and Transfer Learning for Battery Life Prediction of Electric Vehicles Based on Real-Road Driving Obd Data and Lab Measurements	Juri	Lim	362j
90	Accurate Surrogate Models for Stochastic Simulations Using Parin: Parameter As Input-Variable	Samira	Mohammadi	362k
91	Cost Optimization of Steel Alloying Elements with Machine Learning Based Jominy Hardness Profile Prediction	Louis	Allen	362l
92	Hybrid, Interpretable Machine Learning for Thermodynamic Property Estimation Using Grammar2vec for Molecular Representation	Vipul	Mann	362m
93	Predicting Activity Coefficients at Infinite Dilution Using Hybrid Residual Graph Neural Networks	Edgar Ivan	Sanchez Medina	362n
94	Improved Performance of Artificial Neural Networks Via Hyperparameter Optimization and Data Augmentation for a Small Number of Data Sets	Pyeong-Gon	Jung	362o
95	Data-Driven Modeling of Complex Nonlinear Systems Using Hybrid Series and Parallel Nonlinear Static – Dynamic Stochastic Neural Networks	Angan	Mukherjee	362p
96	Modeling Dynamics of Material Flows in Coupled Industrial Processes Using Data Driven System Identification	William	Farlessyost	362r
97	Developing Risk Assessment Framework for Wildfire in the United States – a Deep Learning Approach	Zhuoran	Zhang	362s
97	Developing Risk Assessment Framework for Wildfire in the United States – a Deep Learning Approach	Pingfan	Hu	362s

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BOARD NUMBER	Title	First Name	Last Name	Paper Number
98	High-Throughput Screening for Identifying Potential Chemical Exposure Scenarios at End-of-Life Stage	Mariano	Martin	362u
99	Experimental Evaluation of the Level Detection in Separators Using Electrical Tomography	Pekka	Kaunisto	362v
100	Cover Cut Based Algorithm for Optimal Sensor Network Design	Arjun	M	362w
101	Failure Stage Classification and Its Application to Predicting Remaining Useful Life of Bearings	Bahareh	Hassani	362y
102	Root Cause Identification Using Cross-Correlation Weighted Lag in Chemical Plants	Abhishek	Bansal	362z
103	Process Monitoring and Online Fault Detection and Diagnosis Using Deep Recurrent Neural Networks on Plant Data	Lucky E.	Yerimah	362aa
104	Digitalization of an Experimental Electrochemical Reactor Via the Smart Manufacturing Innovation Platform	Berkay	Citmaci	362ab
105	Physics-Based Penalization for Hyperparameter Optimization in Gaussian Process Regression	Jinhyeun	Kim	362ac
107	Multi-Rate Data-Driven Models for Lactic Acid Fermentation - Parameter Identification and Prediction	Satish	Parulekar	362q
109	Ensemble Learning for Fault Diagnosis in Chemical Processes: Fusion of Results through a K-Nearest Neighbors Algorithm	Rajagopalan	Srinivasan	362x
109	Ensemble Learning for Fault Diagnosis in Chemical Processes: Fusion of Results through a K-Nearest Neighbors Algorithm	Bairi	Sai Vasista	362x

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BOARD NUMBER	Title	First Name	Last Name	Paper Number
	# 363 - Interactive Session: Systems and Process Control			
	Tuesday, November 15, 2022 3:30 PM - 5:00 PM			
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114	Selection of Self-Optimizing Controlled Variables Using Principal Component Analysis	Nabil	Magbool Jan	363d
115	Cost-Optimal Multi-Effect Mechanical Vapor Recompression Evaporation Configuration in Pulp and Paper Industry	Yurim	Kim	363a
116	Process Operability Mapping Using Neural Networks	Karan	Waghela	363c
117	A Data-Driven Dynamic Modeling Methodology Based on POD/Oed/ANNs Method for Large-Scale Dynamic Systems	Weiguo	Xie	363e
118	Machine Learning and System Identification for Dynamical Systems: A Comparative Review	Akhil	Ahmed	363f
119	Data Driven Discovery of Chemical Reaction Kinetics	Md	Rizwan	363g
120	Comparing Reinforcement Learning and Bayesian Optimization for Tuning MPC Policies	David	Pérez-Piñeiro	363h
121	CFD Modeling of Gravity Separator with PID Interface Controller	Chang Kai	Wu	363i
122	Modelling of Fluid Flow and Mass Transfer in a Multi-Channel Microfluidic Reactor Using Computational Fluid Dynamics.	Oluwaseyi	Ayeni	363j
123	Multiscale Modeling and Control of Spray Coating of Quantum Dots	Niranjan	Sitapure	363k
124	Matrix Non-Structural Model and Its Application in Heat Exchanger Network without Split Streams	Ding Hao	Li	363l
125	Continuous and Discrete Control of Flow Networks	Varghese	Kurian	363m
126	Nonlinear Model Predictive Control for the Dividing Wall Column	Xing	Qian	363o
127	Model Predictive Control Considering Stochastic Heat Generation for Thermal Management of Electric Vehicle	Hyein	Jung	363q
128	Data-Gathering Lyapunov-Based Economic Model Predictive Control: Considering Interpretability and Physics-Based Model Selection	Henrique	Oyama	363t
129	Tuning MPC through System-Level Parameterization and Inverse Optimization	Wentao	Tang	363u
130	Online Impedance Analysis Using Chirp Signals in Linear and Non-Linear Systems	Rigved	Samant	363v
131	Directed Randomization to Detect for Cyberattacks on Nonlinear Systems Under Lyapunov-Based Economic Model Predictive Control	Keshav	Kasturi Rangan	363x
132	Pipelines Multi-Product Scheduling and Delivering By Model Predictive Control	Lu	Zhang	363y
133	Constraint-Dropping in Cutting-Set Based Robust Optimization: Enabling Robust Heat Pump Allocation	Tom	Savage	363z
134	Modeling and Predictive Control of the Coffee-Ring Effect in Coalescing QD-Droplets	Omkar	Newalkar	363aa
135	Data-Driven ARX Models with Measurable Disturbances for Model Predictive Control (MPC) of Crop Irrigation	Jisung	Jang	363ac

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BOARD NUMBER	Title	First Name	Last Name	Paper Number
136	Adaptive Economic Model Predictive Control for Batch Processes: Application to Rotational Molding Process	Aswin	Chandrasekar	363ad
137	Online Data-Driven Closed-Loop Model Predictive Control of Nonlinear Systems Using Artificial Neural Networks	Andrew	Branen	363ae
110	A New MILP Formulation for Scheduling Cleaning in Heat Exchanger Networks Consisting of Multi-Pass Heat Exchangers	Parag	Patil	363w
110	A New MILP Formulation for Scheduling Cleaning in Heat Exchanger Networks Consisting of Multi-Pass Heat Exchangers	Babji	Srinivasan	363w
110	A New MILP Formulation for Scheduling Cleaning in Heat Exchanger Networks Consisting of Multi-Pass Heat Exchangers	Rajagopalan	Srinivasan	363w
111	Operator's Eye Gaze Analytics for Evaluating Usability of Human Machine Interfaces in Process Control Applications	Rajagopalan	Srinivasan	363ab
111	Operator's Eye Gaze Analytics for Evaluating Usability of Human Machine Interfaces in Process Control Applications	Mohammed Aatif	Shahab	363ab
111	Operator's Eye Gaze Analytics for Evaluating Usability of Human Machine Interfaces in Process Control Applications	Babji	Srinivasan	363ab

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	# 364 - Interactive Session: Systems and Process Design			
	Tuesday, November 15, 2022 3:30 PM - 5:00 PM			
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BOARD NUMBER	Title	First Name	Last Name	Paper Number
139	Modeling and Analysis of the Production of Formaldehyde from Methanol	Omar	Almaraz	364a
140	Comparing Formulations for Global Flowsheet Optimization with Simultaneous Heat Integration	Dominik	Bongartz	364d
141	Optimizing Resilience in the Assessment of the Water-Energy-Food Nexus	Jesus Manuel	Nuñez Lopez	364e
142	Finite Element Refinement and Selection on the Integration of Design and Control: A Hamiltonian Function-Profile-Based Approach.	Oscar	Palma-Flores	364f
143	Profit Distribution in Interplant Heat Integration Using a Hybrid Optimization Approach	Francisco Javier	López Flores	364g
143	Profit Distribution in Interplant Heat Integration Using a Hybrid Optimization Approach	Luis Fernando	Lira-Barragán	364g
144	A Mass Integration Model between Hydraulic Fracturing Processes and a Power Plant	Luis	Lira-Barragan	364c
145	Solvent Mixture Design Using COSMO-RS Descriptors and Molecular Simulations	Jianping	Li	364h
146	Development of a Resilience Model for the Analysis of Process Systems at the Early Design Stage	Joan	Cordiner	364i
61	Towards an Integrate Field Wide Production Optimization Approach for Upstream Field Recovery	Shakeel	Ramjanee	364b

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BOARD NUMBER	Title	First Name	Last Name	Paper Number
	# 365 - Interactive Session: Systems and Process Operations			
	Tuesday, November 15, 2022 3:30 PM - 5:00 PM			
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62	Towards an Integrated Field Wide Production Optimization Approach for Upstream Hydrocarbon Recovery	Shakeel	Ramjanee	365c
149	Feedback State-Space Mapping Framework for Dynamic Operability Analysis	San	Dinh	365a
150	Mixed-Integer Adjustable Robust Optimization Under Exogenous Uncertainty	Byungjun	Lee	365b
151	New and Efficient Interval Sampling Method for Use of P-Boxes in Off-Line Quality Control	Urmila	Diwekar	365d
152	System-Wide Anomaly Detection By Single Value Using Mscred in MEG Regeneration Pilot Plant	Nayoung	Lee	365h
153	Multiperiod Generalized Disjunctive Programming Optimization in Idaes: Simultaneous Design and Operation of an Integrated Energy System	Edna	Rawlings	365i
113	A Reinforcement Learning Approach for Optimal Scheduling of Multiproduct Batch Plants	Nabil	Magbool Jan	365f
108	Development of Artificial Intelligence Based Models for Biomass Gasification	Satish	Parulekar	365g

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366 - Poster Session: Chemical Engineering Education

Tuesday, November 15, 2022 3:30 PM - 5:00 PM

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BOARD NUMBER	Title	First Name	Last Name	Paper Number
Student Learning and Assessment				
155	Gamification of Learning: Designing a Safety Assessment Card Game	Seng Hoe (billy)	Hue	366a
156	The Oral Exam – an Alternative Approach to Assessment	J. Patrick	Abulencia	366b
157	Data-Driven Analysis of Learning Behavior within a Student-Led Chemical Engineering Wiki	Thomas Nok Hin	Cheng	366c
Educational Tool Development				
158	Making Unit Operations an Immersive Experience through Augmented Reality	Jacob	Crislip	366d
Broadening Participation				
159	Translating DNA Origami Nanotechnology to Middle School, High School, and Undergraduate Laboratories	Anjelica	Kucinic	366e
160	Sense of Belonging within Chemical Engineering and Its Impacts upon Retention	Duncan	Mullins	366f
161	Graduate Involvement in Vertically Integrated Projects for Biomaterials Education Research	Alec	Svenson	366g
162	Increase Recycle to Reduce the Purge – a System to Improve Curriculum Retention	John	Wagner	366h
163	Developing a Framework to Examine Women STEM Faculty's Participation in Entrepreneurship Education Programs	Aida	López Ruiz	366i
164	Self-Efficacy in First-Year STEM Majors Correlates with Academic Progression	Edward	Gatzke	366j
Transport and Modeling				
165	Using Matlab, Simulink, and Simscape in Chemical Engineering Fluid Mechanics Courses	Aycan	Hacioglu	366k
166	Ocular Drug Delivery and Unsteady-State Mass Transfer: A Project-Based Learning Approach Using Comsol Multiphysics	Daniel	Lepek	366l
Laboratory Courses				
167	Development of 3D Printed Desktop Learning Module for Learning Packed and Fluidized Bed Concepts	Zeynep	Durak	366m
168	A Hands-on Experience to Study Membrane Technology Developed By Undergraduate Chemical Engineering Students	Andie	Veeder	366n

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	# 367 - Poster Session: Thermodynamics and Transport Properties (Area 1A)			
	Tuesday, November 15, 2022 3:30 PM - 5:00 PM			
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BOARD NUMBER	Title	First Name	Last Name	Paper Number
171	Evaluation of Vapor-Liquid and Solid-Liquid Equilibria for Systems Containing Tetrahydrofuran and Dimethyl Carbonate Using Asog Model	Katsumi	Tochigi	367a
172	A Note on Selectivity of Co-Solvent for Drug Production Process Using Ternary Infinite Dilution Activity Coefficient –Etodolac + Water + Co-Solvent System –	Katsumi	Tochigi	367b
173	Enthalpy of Mixing and Liquid Structure of Primary and Secondary Alcohols	Chun-Kai	Chang	367c
174	Volumetric and Acoustic Properties of Saccharides in Aqueous Solutions Containing Polyethylene Glycols (PEGs)	Ricardo	Torres	367d
175	Sustainable Methane Storage Using Gas Hydrates with Superabsorbent Polymers (SAPs) and Tetrahydrofuran (THF) Under a Quiescent System	Dong Woo	Kang	367e
176	Thermodynamics Modeling Employing the Compound Energy Formalism with Novel Complementary Use of Experimental and First Principles Data: A Case Study of $Ba_{1-x}Sr_xFeO_{3-\delta}$	Steven	Wilson	367f
177	Effect of Cationic Species on the Activity and Inhibition Performance of NO_2^-/NO_3^- Corrosion Inhibitors	Ahmed	Mohamed	367g
178	Development of the Hydrocarbon Polymer Electrolyte Membranes and the Modeling Analysis By Using Molecular Dynamics	Hyunseo	Park	367h
179	Modifying Reactor Structure to Improve Efficiency from a Heterogeneous Approach	Kei	Sakurai	367i
180	Study of Granular Flow in a Wedge-Shaped Hopper Using DEM Simulations	Afroz	Momin	367j
181	Rheological Characteristics of Tetra-n-Butylammonium Bromide Hydrate As a Thermal Energy Carrier	Ponnivalavan	Babu	367k

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 # 368 - Poster Session: Nanoscale Science and Engineering Forum

Tuesday, November 15, 2022 3:30 PM - 5:00 PM

North Hall E, Phoenix Convention Center

BOARD NUMBER	Title	First Name	Last Name	Paper Number
184	Surface-Mediated Assembly of Site-Modified Green Fluorescent Protein into Two-Dimensional Nanosheets As a Platform for Hierarchical Materials Fabrication	Nada	Naser	368a
185	A Machine Learning Study on the Result of Polarizable Molecular Dynamics of Ionic Liquid-Based Solid Polymer Electrolytes for Li^+-Ion Batteries By Graph Dynamical Networks	Chanui	Park	368b
186	Lithium Ion Transport Mechanism in PYR_{14}tfsi/PEO Branched Nanopore System: A Polarizable Molecular Dynamics Study	Sebin	Kim	368c
187	Improvement of Storage Stability of mRNA Vaccine Using Lipid Based Drug Delivery System	Minsub	Chung	368d
188	Synthesis of Metal-Organic Frameworks (MOFs) and Evaluation of Their Toxicological Profiles.	Olivia	Rose	368e
189	Protein Templated Core/Shell Nanostructures for Photothermal Therapy and SERS Mediated Intracellular ROS Detection	Animesh	Pan	368g
190	Synthesis of Near-Infrared Pigments for Novel Sensor Applications	John	Clark	368i
60	Diffusion Growth Mechanism of Penta-Twinned Ag/Cu Nanowires: Multiscale Theory	Jianming	Cui	368f
191	Optimizing Composition and Solar Light Conditions for the Reversible Diels-Alder Reaction in Titanium Nitride Nanoparticle-Laden Epoxy	Kavon	Mojtabai	368h
191	Optimizing Composition and Solar Light Conditions for the Reversible Diels-Alder Reaction in Titanium Nitride Nanoparticle-Laden Epoxy	Madeline	Finale	368h
191	Optimizing Composition and Solar Light Conditions for the Reversible Diels-Alder Reaction in Titanium Nitride Nanoparticle-Laden Epoxy	Arnob Dipta	Saha	368h
191	Optimizing Composition and Solar Light Conditions for the Reversible Diels-Alder Reaction in Titanium Nitride Nanoparticle-Laden Epoxy	Sanchari	Chowdhury	368h

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369 - Poster Session: NSEF Graduate Student Poster Competition

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BOARD NUMBER	Title	First Name	Last Name	Paper Number
192	Development and Characterization of Recyclable Epoxy/Refractory Plasmonic Nanoparticles for Additive Manufacturing	Arnob Dipta	Saha	369c
193	Upgrading Food Waste to High Commercial Value Chemicals	Yagya	Gupta	369a
194	Controlling Metal Nanoparticle Size Distribution through Microreactor Residence Time Distribution	Faiz	Khan	369b
195	Development of Magnetic Nanoparticles and Nanocomposites for Environmental and Biomedical Applications	Pranto	Paul	369d
196	Development of Methods for Precise, Multifactor Tuning of Shell Morphology on Silica-Encapsulated Gold Core-Shell Nanoparticles	Ellis	Hammond-Pereira	369f
197	NSEF Poster Session: Computational Studies on the Structural Properties of Square Colloids with Offset Magnetic Dipoles	Matthew	Dorsey	369g

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# 370 - Poster Session: Bioseparations				
Tuesday, November 15, 2022 3:30 PM - 5:00 PM				
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BOARD NUMBER	Title	First Name	Last Name	Paper Number
198	Demonstrating the Scale up of Single-Use Centrifugation/Washing/Media Exchange for Cell Cultures at the Bench, Pilot Plant and Manufacturing Bioreactors.	David	Richardson	370b

# 371 - Poster Session: Fundamentals and Applications of Adsorption and Ion Exchange				
Tuesday, November 15, 2022 3:30 PM - 5:00 PM				
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BOARD NUMBER	Title	First Name	Last Name	Paper Number
Gas-phase Applications of Adsorption				
200	Adsorption Equilibria and Kinetics of CO_2, CO, CH_4, N_2, O_2, and H_2 on Silica-Based Adsorbents	Jun-Ho	Kang	371e
201	Guide to COF Adsorbent for Ammonia-based Green Hydrogen with Multi-scale Evaluation Approach	Nahyeon	An	371a
202	Amine-Modified Silica Materials for Direct Carbon Dioxide Capture from the Atmosphere	Amirjavad	Ahmadian Hosseini	371b
203	Adsorption Mechanism of Ultra-Low Concentration H_2s and THT in CH_4 on Zeolites in the Presence of CO_2	Gina	Bang	371c
204	A New Dynamic Vapor Sorption Instrument for the Investigation of Water Sorption on Porous Materials	Thomas	Paschke	371d
205	Performance Evaluation and Comparison of Conventional and Emerging Adsorbents in Their Applications to a CO_2 Capture Vacuum Pressure Swing Adsorption (VPSA) Process	Yixuan	Zhang	371f
206	Adsorbents for Selective Adsorption of VOC Biomarkers from Simulated Breath	Ojuolape	Oghenetega	371g
207	Epoxide-Modified Amine-Based CO_2 Adsorbent for Direct Air Capture	Yao	Ma	371h
208	Boosting Volumetric and Gravimetric H2 Storage Capacity of Carbon-Based Sorbents Through Tuning Surface Chemistry and Densification Approaches	Ruthra	Murugavel	

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BOARD NUMBER	Title	First Name	Last Name	Paper Number
Adsorbent Materials				
209	Porous Carbon from Non-Recyclable Plastic Wastes	Brian	Hoffman	371j
210	Direct Ink 3D Printing of Porous Carbons	Marisa	Comroe	371k
211	Diffusion Studies of Hydrocarbons in Ill-Crystallized or Desilicated ZSM-5 Catalysts	Celio	Cavalcante	371l
212	Understanding Fluid Phase Behavior in Geometrically Disordered Mesoporous Materials	Henry R. N. B.	Enninful	371m
213	Boosting Volumetric and Gravimetric H_2 Storage Capacity of Carbon-Based Sorbents Through Tuning Surface Chemistry and Densification Approaches	Ruthradharshini	Murugavel	371r
Liquid-phase Applications of Adsorption				
214	Synthesis of Mussel-Inspired Polydopamine Mediated with Ionic Liquid As a Sustainable Adsorbent for the Selective Removal of Anionic Pollutants for Wastewater Applications	Botagoz	Zhuman	371o
215	Investigating Alkali-Activated Fly Ash Based Materials As Adsorbents for Heavy Metal Sorption	Monday	Okoronkwo	371p
216	Hyper-Crosslinked Tetraphenylboron (TPBx) As a Versatile Platform Material for the Development of Sorbents for Various Metal Ions	Grace	Nisola	339c
217	Phosphorous-Doped Mesoporous Carbon As an Efficient Adsorbent for the Recovery of Neodymium (III) Metal Ion from an Aqueous Medium	Gebremedhn T.	Gebremichael	143d
218	Demonstration of Iodine Removal Efficiency of MOF-Based Sorbents from Nuclear Waste Solutions in the Presence of Interfering Ions	Turki	Alghamdi	371q

#372 - Poster Session: General Topics on Separations

Tuesday, November 15, 2022 3:30 PM - 5:00 PM

North Hall E, Phoenix Convention Center

BOARD NUMBER	Title	First Name	Last Name	Paper Number
219	Hybrid Heat-Integrated Design Alternatives of Dimethyl Carbonate Reactive Distillation	Minyong	Lee	372b
220	A Low-Temperature Hollow Fiber Membrane Reactor for Propane Dehydrogenation	Lu	Liu	372c
221	The Technology Development in Magnesium Production and Separation	Lucas	Arndt	372d
222	Selective Recovery of Au^{3+} *via* Complexation-Reduction Capture and Release By Thermo-Responsive P(NIPAM-co-15TCE-4)@SiO_2 Nanoparticles.	Hiluf Tekle	Fissaha	372e
223	$Co_{1-x}[Fe(III)(CN)_6]$/Ag for Electrochemical Recovery of Cobalt Ion from Spent Nickel Metal Hydride Batteries	Hana G.	Zeweldi	372g
224	Selective Adsorption of Chlorofluorocarbons (CFC) and Hydrochlorofluorocarbons (HCFC) in Hydrofluorocarbon's (HFC) Using Adsorbent Supported Metal Oxide.	Anup Kumar	Doraiswamy	372i
225	Project Earth (Environmentally Applied Research Towards Hydrofluorocarbons) Ionic Liquids Approach	Kalin R.	Baca	372j
226	Phase Equilibria for HFC-32, HFC-125, and Binary Mixtures (R-410A) with a Variety of Ionic Liquids	Kalin R.	Baca	372p
227	Impact of Wafer Chemistry on Electrodeionization Removal and Selectivity	Leticia	Santos de Souza	372k
228	Estimation of Supersaturation in Pressure-Driven Supersaturated Gas-Liquid Systems	Sushobhan	Pradhan	372l
229	Identification of the Innovative Separation Technique for Sustainable Society	Akanksha	Prasad	372m
230	Understanding Separation Mechanisms of Monoatomic Gases, Such As Kr and Xe, Via DD3R Zeolite Membrane Using Molecular Dynamics	Bandar	Bashmmakh	372o
231	Separation of Dispersed Water from ULSD Using a Wire Mesh Electrowet Coalescer	Mohammad	Assaleh	372q
232	Barriers to Electrodialysis Implementation: Maldistribution and Its Impact on Resistance and Limiting Current Density	Jack	Ledingham	372r
233	Utilizing Capillary Isoelectric Focusing to Identify Uremic Toxins in the Urine of Chronic Kidney Disease Patients	Haley	Duncan	372s
234	Porous Ionic Liquids: Theoretical and Experimental Research	Hongping	Li	372t
235	Eutectic Ionic Liquids for Efficient Gas Separation	Guokai	Cui	372u

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	# 373 - Poster Session: Membrane Separations			
	Tuesday, November 15, 2022 3:30 PM - 5:00 PM			
	North Hall E, Phoenix Convention Center			
BOARD NUMBER	Title	First Name	Last Name	Paper Number
	Liquid phase separations			
241	Designing, Preparing and Characterizing Alkali Treated Graphitic Carbon Nitride Thin Film Composites (TFC) Membranes for Efficient Dye Salty Water Separation.	Ameya	Tandel	373a
242	Membrane Material Development for Spaceflight Wastewater Applications	Elisabeth	Thomas	373b
243	Effect of Ionic Liquid Cations and Anions on the Cellulose Acetate Membrane Characteristics and Performance for Water Treatment	Atta Ur	Razzaq	373c
244	2D Assembly of Graphene Oxide Nanoribbon *Via* Slot-Die Coating and Its Application for Organic Solvent Nanofiltration	Ji Hoon	Kim	373d
245	Microwave-Assisted Nanoporous Multilayer Graphene Membrane with Ultrafast Organic Solvent Nanofiltration	Junhyeok	Kang	373f
246	Treatment of Produced Water Using Sand Filtration and Ultrafiltration Using Modified α-Alumina Membranes	Anirban	Ghosh	373g
247	Production of Nanofiber Membranes Using Centrifugal Spinning	Maryam	Amouamouha	373h
248	Ceramic Membrane Synthesis, Application and Characterization	Tejay	Lanjewar	373i
249	Progress in the Development of Membranes for Pressure Retarded Osmosis Process	Dr. Syed	Zaidi	373k
250	Separation of Olefin-Paraffin Mixtures with Optiperm^{TM} customized Amorphous Fluoropolymer Membranes	William	Charlton	373l
251	Implications of Shear and Cation Choice on Dynamics of Nonliving Natural Organic Matter	Kathlyn	Mealio	373j
252	Investigation of Correlation Between Membrane Characteristics and Rejection Rate of Ions	Kiwoong	Kim	373k

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BOARD NUMBER	Title	First Name	Last Name	Paper Number
**Vapor phase separations - Materials**			
253	Petrified Hollow Fiber Membranes with Hierarchical Pores	Ching-En	Ku	373m
254	Improving Propylene/Propane Separation Performances of Polycrystalline ZIF-8 Membranes Via Additive-Assisted Microstructural Modification	Donga	Kang	373n
255	Dehydrated Channel Protein-Based Biomimetic Membranes with High Breathability and Protective Capability	Hyeonji	Oh	373o
256	Effect of Grafting Density and Sidechain Length on Mechanical and Gas Transport Properties of Poly(ladder) Romps	Sherrie	Qian	373p
257	Unexpectedly High Propylene-Selective Mixed-Matrix Membranes with Facile in-Situ ZIF-8 Filler Formation Process	Yinying	Hua	373q
258	Carbon Molecular Sieve Gas Separation Membranes Pyrolyzed from Aromatic Barrier Polymers	Gaurav	Iyer	373r
259	Separation of HFC-32, HFC-125, HFC-134a, HCFC-22, and HFO-1234yf Using Copolymers of Perfluoro(butenyl vinyl ether) and Perfluoro(2,2-dimethyl-1,3-dioxole)	Abby	Harders	373s
260	Iptycene-Based Polybenzimidazole Membranes for H_2/CO_2 Separation	Mengdi	Liu	373t
261	Application of 2^6-Factorial Design Optimization for PVA Based Membrane Synthesis for CO_2/N_2 and CO_2/CH_4 Separation	F Handan	Tezel	373w
262	Feasibility Study of Membrane Reactor for Reverse Water Gas Shift By ZSM-5 Zeolite Membrane	Motomu	Sakai	373x
**Vapor phase separations - Processes**			
263	Process Design and Optimization of Membrane-Cryogenic CO_2 Capture Process for Industrial CO_2 Emissions	Mun-Gi	Jang	373z
264	Elucidating Key Factors Dominating Natural Gas Sweetening Efficiency of Membranes	Yang	Liu	373aa
265	Dynamic Modeling and Simulation of a Membrane Contactor for CO_2 Absorption	Wanderson	Passos	373ab
266	Respirator Cartridge Performance Testing for Chemicals of Potential Concern (COPC) at Higher Chemical Vapor Concentrations	Satish	Nune	373ac
267	Integrated Module Array with Facilitated Transport Membranes for Enhanced H_2 Recovery from Syngas	Yang	Han	373y

BOARD NUMBER	Title	First Name	Last Name	Paper Number
	# 374 - Poster Session: Separations Division			
	Tuesday, November 15, 2022 3:30 PM - 5:00 PM			
	North Hall E, Phoenix Convention Center			
268	Carbon Capture from Residual Emissions Enabled By Facilitated Transport Membranes	Yang	Han	374i
269	Optimal MEA/Dipa/Water Blending Ratio for Minimizing Regeneration Energy in Absorption-Based Carbon Capture Process: Experimental Solubility and Thermodynamic Modeling	Mun	Jihun	374b
270	Optimal MEA/Dipa/Water Blending Ratio for Minimizing Regeneration Energy in Absorption Based Carbon Capture Process: Experimental Solubility and Thermodynamic Modeling	Mun	Jihun	374e
271	Synthesis and Characterization of CO_2-Selective Membranes with Poly(ethylene formamidine)	Jingying	Hu	374c
272	Responsive Membranes for Enhanced Capture and Detoxification of Water and Air Pollutants	Rollie	Mills	374d
273	Precise Control of Pore Size of Clinoptilolite and Separation of N2 from CH4	Hiroshi	Okaniwa	374f
274	Electrospun Polymer Fibers for Carbon Capture of CO_2	Edward	Huang	374h
275	Application of Calcium Oxide-Based Bifunctional Catalytic Sorbent to Hydrogen Production	Pilseok	Kim	374j
276	Ca-Al Hydrotalcite-Based Mixed-Metal-Oxide for High-Temperature Carbon Dioxide Adsorption	Kuei Tan	Lee	374k
277	Selective Removal of Cs^+ in Acidic Nuclear Water Waste Using Epoxy Resins	Erwin	Escobar	374l
278	Tunable H_2s/CO_2 Separation Using Sterically Hindered Amine Membranes	Shraavya	Rao	374m
279	Separation of Refrigerant R-410A Using Porous Materials: Thermodynamic Modeling and Breakthrough Experiments	Andrew	Yancey	374n
280	Evaluating Transport Factors to Understand Electrochemical Nutrient Removal and Recovery from Synthetic Animal Wastewater	Sana	Heydarian	374o
281	Intensified Water Purification Via Closed Loop Carbon Dioxide-Mediated Diffusiophoresis	Esai	Lopez	374p
282	Effect of Co-Ions on O_2 Gas Transport Properties of Cross-Linked Poly(ethylene oxide)	Taliehsadat	Alebrahim	374q

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BOARD NUMBER	Title	First Name	Last Name	Paper Number
283	Synthesis and Characterization of Multi-Ionic Block Copolymers for Chemical and Biological Protective Clothing Applications	Gilberto	Ramos Rivera	374r
284	Separation of Refrigerant Mixtures Using Extractive Distillation with Ionic Liquid Entrainers	Mark B.	Shiflett	374s
285	Energy Efficient Advanced Separation Process of Solvent Mixture (Xylene, Butyl Acetate and Methyl Ethyl Ketone) Recovery/Re-Processing for Paint Industry	Abdur	Rehman	374u
286	CFD-PBM Simulation of Nickel-Manganese-Cobalt Hydroxide CO-Precipitation in CSTR	Daniele	Marchisio	374v
287	Energy-Efficient Process of Advanced Separation Technologies of Solvent Mixture (Xylene, Butyl Acetate and Methyl Ethyl Ketone) Recovery/Re-Processing for Paint Industry	Muhammad	Haider	374x
199	Performance Analysis of a Multi-Bed PSA Process Using Silica-Based Adsorbents for CO_2 Capture from Off-Gas in Iron and Steel Industry	Jun-Ho	Kang	374g

	# 375 - General Poster Session in Sensors			
	Tuesday, November 15, 2022 3:30 PM - 5:00 PM			
	North Hall E, Phoenix Convention Center			
BOARD NUMBER	Title	First Name	Last Name	Paper Number
289	Pd-Nanoparticle Enabled Optical Fiber Hydrogen Sensor for Subsurface Storage Conditions	Daejin	Kim	375a
290	Reshaping Molecularly Imprinted Polymers for Robust Sensing Performance	Cameron	Malloy	375b
291	Dynamic Complex Emulsion Based Multiplexed Sensing Array for Environmental Contaminants Detection	Baishali	Barua	375c
293	Stress Sensor Synthesis Using Electropolymerized Molecularly Imprinted Polymers	Grace	Dykstra	375d
294	Enzymatic Electrochemical Sensing for Fish Freshness Using Macro-Porous NiO Electrodes	Anuja	Tripathi	375e
295	Construction of a Sensor for Rapid and Online Measurement of Dissolved Methane in Bioreactor Systems	Robert	Bertrand	375f

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