

Computational Molecular Science and Engineering Forum 2022

Held at the 2022 AIChE Annual Meeting

Phoenix, Arizona, USA
13-18 November 2022

ISBN: 978-1-7138-7905-3

Printed from e-media with permission by:

Curran Associates, Inc.
57 Morehouse Lane
Red Hook, NY 12571



Some format issues inherent in the e-media version may also appear in this print version.

Copyright© (2022) by AIChE
All rights reserved.

Printed with permission by Curran Associates, Inc. (2023)

For permission requests, please contact AIChE
at the address below.

AIChE
120 Wall Street, FL 23
New York, NY 10005-4020

Phone: (800) 242-4363
Fax: (203) 775-5177

www.aiche.org

Additional copies of this publication are available from:

Curran Associates, Inc.
57 Morehouse Lane
Red Hook, NY 12571 USA
Phone: 845-758-0400
Fax: 845-758-2633
Email: curran@proceedings.com
Web: www.proceedings.com

TABLE OF CONTENTS

APPLICATIONS OF MOLECULAR MODELING TO STUDY INTERFACIAL PHENOMENA I

9a Atomistic-Level Insights into the Interfacial Interactions Between Amyloid-Beta and Phospholipid Bilayers for the Treatment of Alzheimer's Disease	1
<i>Bailey Zinger, Joel L. Kaar, Kayla Sprenger</i>	
9c Computational Discovery of Plastic-Binding Peptides for Microplastic Remediation.....	2
<i>Michael Bergman, Xingqing Xiao, Carol Hall</i>	
9d Computational Investigation of Bijels as Separation Systems.....	3
<i>Marco Tilio Portella, Xuan Duy Thao Nguyen, Dimitrios Papavassiliou</i>	
9e Adsorption of Trace Metal Contaminants from Coal-Derived Syngas on Metal Surfaces and Novel Bimetallic Adsorbents.....	4
<i>Dwijraj Mhatre, Divesh Bhatia</i>	
9f Vapor-Liquid Equilibrium and Nucleation Studies of Water from First Principles-Based Machine Learning Models.....	6
<i>Maria Carolina Nicola Barbosa Muniz, Roberto Car, Athanassios Panagiotopoulos</i>	
9g Metastable Liquid-Liquid Criticality in Supercooled Wail Water	7
<i>Jack Weis, Athanassios Panagiotopoulos, Pablo Debenedetti</i>	
9h Molecular Dynamics of Ethoxylated Surfactants in Water/N-Heptane Interface	8
<i>Arthur M. Luz, Gabriel D. Barbosa, Thiago Jose Pinheiro Dos Santos, Carla L. M. Camargo, Frederico W. Tavares</i>	
9i Dynamic Molecular Switching for Environmentally Adaptive Surfaces.....	9
<i>Nicholas Craven, Chris R. Iacovella, G. Kane Jennings, Clare McCabe</i>	
9j Interactions of Cellulosic Oligomers with Different Crystallographic Surfaces of Cellulose Nanocrystals Through Molecular Simulation.....	10
<i>Naveen Vasudevan, Dongyang Li, Li Xi</i>	

POSTER SESSION: COMPUTATIONAL MOLECULAR SCIENCE AND ENGINEERING FORUM

360a Exploring Canyons in Soft and Glassy Energy Landscapes Using Metadynamics	11
<i>Amruthesh Thirumalaiswamy, Robert Riggeman, John C. Crocker</i>	
360c the Role of Heteroatom Placement and Chain Branching on Quaternary Ammonium Salts for Phase Transfer Catalysis.....	12
<i>Brooks Rabideau, Rome Parker</i>	
360d Investigating the Effect of Oxidic Functional Group on Graphene Oxide-Molybdenum Disulfide Heterostructures as Anode for Sodium-Ion Battery	13
<i>Wonmyung Choi, Byungchan Han</i>	

360e a Study on the Ionic Conductivity Improvement Mechanism of Halospinel Li ₂ Sc ₂ /3Cl ₄ by Variable Li and Dopant Concentration	14
<i>Suseong Hyun, Hoje Chun, Minjoon Hong, Byungchan Han</i>	
360f Redox Behavior of Single Atom Catalysts for the Upgrading of Plastic Waste-Derived Species.....	15
<i>Jeremy Hu, Eun Mi Kim, Mikyung Hwang, Michael J. Janik, Hilal Ezgi Toraman, Konstantinos Alexopoulos</i>	
360g Revisiting Nanoparticle Interactions for Effective Nanofluid Modeling and Simulation.....	16
<i>Jee-Ching Wang</i>	
360h the Molecular Simulation Design Framework (MoSDeF): New Capabilities	17
<i>Co D. Quach, Justin Gilmer, Umesh Timalsina, Nicholas C. Craven, Christopher Iacovella, Clare McCabe, Peter Cummings</i>	
360i Microbubbles as Non-Invasive Targets for Blood Brain Barrier Disruption: an in Silico Investigation	18
<i>Bailey Zinger, Payton Martinez, Kendra Kreienbrink, Mark A. Borden, Kayla Sprenger</i>	
360j Deep Reinforcement Learning as a Tool to Enable Coarse Grained Vaccine Models	19
<i>Jonathan Faris, Daniel Orbidan, Brenden Petersen, Kayla Sprenger</i>	
360k Optiboost: a Method for Choosing a Safe and Efficient Boost for the Bond-Boost Method in Accelerated Molecular Dynamics (AMD) Simulations with Hyperdynamics (HD)	20
<i>Jianming Cui</i>	
360l Toward Accurate and Transferable Coarse-Grained Peptide Models Using Data-Driven Approaches.....	21
<i>Luc Christians, Alexander J. Pak</i>	
360m Predicting Quantum-Accurate DNA Electron Densities and Forces with Equivariant Neural Networks	22
<i>Alex Lee, Joshua A. Rackers, William P. Bricker</i>	
360n Elucidating Ethylene Hydrogenation on Site Isolated Intermetallic Catalysts	23
<i>Angela Nguyen, Griffin A. Canning, Michael J. Janik, Robert Rioux</i>	
360o Electron Density Prediction with Graph Neural Networks on Large Catalyst Datasets	24
<i>Ethan Sunshine, Muhammed Shuaibi, Zachary Ulissi</i>	
360p Exceptional Stability of Gd-Doped UO ₂ Against Surface Oxidation: First-Principles Study.....	25
<i>Minjoon Hong, Byungchan Han</i>	
360q Explaining Improvements in Li-Ion Battery Performance by Atomic Layer Deposition of Alumina Using Molecular Dynamics Simulation.....	26
<i>Julie A. Nguyen, Abigayle Becker, Krishan Kanhaiya, Alan Weimer, Hendrik Heinz</i>	
360s Positive Unlabeled Learning of Peptide Properties.....	27
<i>Mehrad Ansari, Andrew White</i>	
360t Elucidating Ligand Selectivity and Partial Agonism Towards Cannabinoid Receptors Using Machine Learning Approaches.....	29
<i>Soumajit Dutta, Balaji Selvam, Austin Weigle, Diwakar Shukla</i>	
360u Molecular Simulations of Protein/Ligand-Mediated Microglial Activation in Alzheimer's Disease	30
<i>Emma Lietzke, Kimberley Bruce, Kayla Sprenger</i>	

360v Coarse-Grained Molecular Dynamics Simulations of ssDNA Loaded Adeno-Associated Virus	31
<i>Tibo Duran, Arani Chanda, Willow Diluzio, Ryan Bellucci, Shivangi Naik, Bodhisattwa Chaudhuri</i>	
360w Design of Pore Wall Chemistry to Control Solute Transport and Selectivity	33
<i>Sally Jiao, M. Scott Shell</i>	
360x Studying Anhydrous Proton Transport on Graphene-Based Materials Using Deep Learning Methods.....	34
<i>Siddarth Achar, Leonardo Bernasconi, Linfeng Zhang, Karl Johnson</i>	
360y the Nuclear and Surface Electrostatic Potential as Descriptors of Chemical Interactions	35
<i>Joakim Halldin Stenlid, Frank Abild-Pedersen</i>	
360z Understanding DNA Hybridization Through Thermodynamics and Kinetics of Abasic Oligomers.....	37
<i>Mike Jones, Brennan Ashwood, Andrei Tokmakoff, Andrew Ferguson</i>	
360aa the Chebyshev Interaction Model for Efficient Simulations (ChIMES): Machine-Learned Interatomic Models for Quantum-Accurate Reactive Simulation	38
<i>Rebecca Lindsey, C. Huy Pham, Nir Goldman, Laurence E. Fried, Sorin Bastea</i>	
360ab Inverse Design of Open Nanocrystal Superlattices Using an Oscillating Pair Potential.....	39
<i>Chase Petix, Michael Howard</i>	
360ac Using Text-Mining and Community Knowledge to Quantify and Engineer Stability in MOFs	40
<i>Aditya Nandy, Heather Kulik</i>	
360ad Electrical Double Layer Capacitance and Polarizability Modeled Using Classical Molecular Dynamics.....	41
<i>Bolton Tran, Scott T. Milner, Michael J. Janik</i>	
360ae Insights of Phenolic Compounds Extraction from an Aqueous Environment Using Natural Deep Eutectic Solvents: Quantum Chemical and Molecular Dynamics Simulation	42
<i>Nikhil Kumar, Tamal Banerjee</i>	
360af Investigating the Electrocatalytic Reduction of 2,4,6-Tri-Nitro-Toluene (TNT) Across Late Transition Metal Surfaces Using Density Functional Theory Methods.....	43
<i>Andrew Wong, Joshua Miller, Brandon Perdue, Michael J. Janik</i>	
360ag Identification of Potential TMPRSS2 Inhibitors by Virtual Screening Using Molecular Docking and Machine Learning	44
<i>Suraj Ugrani</i>	
360ah Self-Assembly of Lobed Colloidal Particles into Porous Morphologies	45
<i>Brunno C. Rocha, Harish Vashisth</i>	
360ai Simulation of Lipid Membranes Using Coarse-Grained Model and Reverse-Mapping	46
<i>Hiroya Nitta, Taku Ozawa</i>	
360aj Determination of Electronic Driving Factor for Selective Adsorption of Arsenic Over Phosphorous Oxoanions by Fe(III)-Crosslinked Chitosan Using DFT	47
<i>Obinna Nwokonkwo, Christopher Muhich</i>	
360an Development and Validation of Non-Bonded Interaction Parameters Between Coarse-Grained Amino Acid Models and Water	48
<i>Esmat Mohammadi, Soumil Joshi, Sanket Deshmukh</i>	

360ak Insights into the Phase Diagram of Pluronic L64 Using Coarse-Grained Molecular Dynamics Simulations.....	49
<i>Mangesh Bhendale, Arpita Srivastava, Jayant K Singh</i>	
360ao Elucidating the Bulk and Interfacial Structure of Ionic Liquids from the Dilute to Concentrated Regimes Using Molecular Dynamic Simulations	50
<i>Lisa Je, Beichen Liu, Matthew Gebbie, Victor Zavala, Reid Van Lehn</i>	
360ap Developing Deep Learning Models to Predict Sigma Profiles of Lignin-Derived Organic Molecules	51
<i>Usman Abbas, Manh Tien Nguyen, Yuxuan Zhang, Jian Shi, Jin Chen, Qing Shao</i>	
360aq Effect of Solvent Quality on Structure and Dynamics of Lignin in Solution	52
<i>Nusrat Jahan, Md Masrul Huda, Neeraj Rai</i>	
360ar Identifying the Stoichiometry of the Metastable Cu ₃ State in Alkaline Electrochemical Systems Using DFT-Based Theoretical Raman Standards	53
<i>Lars Ostervold III, Bolton Tran, Maxwell Wetherington, Konstantinos Alexopoulos, Lauren F. Greenlee, Michael J. Janik</i>	
360as Bayesian Forcefield Driven Monte Carlo and Molecular Dynamics Simulations of O and Cl Promoted Silver Surface Reconstructions	55
<i>Anna Sviripa, Ching-Tien Chen, David Flaherty, Christopher Paolucci</i>	
360at Explosive Mechanochemistry: Foundations for Strength-Aware Chemical Kinetics	57
<i>Matthew Kroonblawd, Brad Steele, Brenden Hamilton, Chunyu Li, Matthew Nelms, Ryan Austin, Laurence E. Fried</i>	
360au Protein Interactions Determined from Computational Methods	58
<i>Gregory Dignon, Barbara Hribar-Lee, Dima Kozakov, Ken A. Dill</i>	
360av a Computational Study for Predicting Stability Differences in Multiple Conformations of the Sars-CoV-2 Frameshifting RNA Element	59
<i>Karim Malekzadeh, Gul H. Zerze</i>	
360aw Comparison of Advanced Sampling Techniques for Atomistic Scale RNA Folding	60
<i>Kosar Rahimi, Gul H. Zerze</i>	
360ax Understanding the Normal Bicontinuous Cubic Phase in Gemini Lyotropic Liquid Crystals in Order to Design Selective Separations	61
<i>Nathanael Schwindt, Subin Sahu, Douglas L. Gin, Richard D. Noble, Michael Shirts</i>	
360ay Parameterization of C, Si, and Ge in the Common Harmonic Form for Molecular Dynamics Simulations.....	62
<i>Katarina Odak, Hendrik Heinz, Alan Weimer</i>	
360az the Role of Antiretroviral Therapeutics as Both Inhibitors and Substrates of P-Glycoprotein	63
<i>Daisy Fuchs, Sahana Balaji, Kayla Sprenger</i>	
360ba Modeling of Photoresist Pattern Formation in EUV Lithography Through Molecular Dynamics Simulations.....	64
<i>Seungtae Kim, Sangwoo Kwon, Won Bo Lee</i>	
360bb Benchmarking Martini 3.0 Force Field for Reproducing Thermodynamic Properties of Biomolecular Condensates	65
<i>Ayush Gupta, Gul H. Zerze</i>	

360bc Understanding Protein Unfolding Under Different Stressors from Molecular Dynamics Simulations.....	66
<i>Yinhao Jia, Janani Sampath</i>	
360bd CCR5-Eriously? Reexamining HIV-1 Tropism Switching with In Silico directed Evolution	67
<i>Jonathan Faris, Bailey Zinger, Brenden Petersen, Kayla Sprenger</i>	
360be Monte Carlo Simulations Predicting Adsorption of 1,4-Dioxane in All-Silica Zeolites	68
<i>Samiha Sharlin, Tyler R. Josephson</i>	
360bf Coarse-Grained Models of Polyetherketoneketone (PEKK) Used to Perform Fusion Weld Simulations and Predict Resulting Mechanical Properties.....	69
<i>Chris Jones, Jenny Fothergill, Rainier Barrett, Eric Jankowski</i>	
360bg Investigating Stable and Active Catalysts for Hydrogen Generation Via Methane Pyrolysis in Molten Media, Using Ab Initio Molecular Dynamics	70
<i>Ojus Mohan, Samir H. Mushrif</i>	
360bh Extending the MolMod Database to Transferable Force Fields	72
<i>Sebastian Schmitt, Gajanan Kanagalingam, Daniel Fröscher, Florian Fleckenstein, Hans Hasse, Simon Stephan</i>	
360bi Mass Transfer Through Vapor-Liquid Interfaces of Binary Mixtures Studied by Non-Stationary Molecular Dynamics Simulations	73
<i>Dominik Schaefer, Jens Staubach, Simon Stephan, Hans Hasse</i>	
360bj Theoretical Investigation of the Coverage Effect on Ni-In Intermetallic Catalysts for Selective Hydrogenation of Acetylene to Ethylene	74
<i>Zahra Almisbaa, Hassan Aljama, Luigi Cavallo, Philippe Sautet</i>	

MACHINE LEARNING FOR SOFT MATERIALS I

622a Inverse Design of Pore Wall Chemistry to Control Solute Transport Through Molecular Simulation Coupled Optimization.....	75
<i>Sally Jiao, M. Scott Shell</i>	
622b Multi-Multimolecular Latent Space Simulations of DNA Hairpin-Duplex Competition.....	76
<i>Mike Jones, Andrew Ferguson</i>	
622c Machine Learning-Enabled Prediction of Electronic Properties of Radical Polymers at Coarse-Grained Resolutions	77
<i>Riccardo Alessandri, Juan J. De Pablo</i>	
622d Machine Learning Guided Discovery of Polymer Membranes for Reducing Greenhouse Gas Emissions	78
<i>Yasemin Basdogan, Zhen-Gang Wang</i>	
622e Sigma Profiles in Deep Learning: Towards a Universal Molecular Descriptor	79
<i>Dinis O. Abrantes, Yong Zhang, Edward Maginn, Yamil Colón</i>	
622f Systematic Investigation of Training Protocols for Machine Learning Derived Interatomic Potentials	80
<i>Nisarg Joshi, Jim Pfaendtner</i>	

622g Application of Machine Learning to Accelerate High-Throughput Molecular Dynamics Screening: a Study of Tribological Properties of Monolayer Films	81
<i>Co D. Quach, Justin Gilmer, Daniel Pert, Akanke Mason-Hogans, Peter Cummings, Clare McCabe</i>	
622h Detecting Transition Boundaries in Molecular Simulations	82
<i>Brandon Butler, Domagoj Fijan, Sharon C. Glotzer</i>	
<u>HONORARY SESSIONS FOR KEITH GUBBINS' 85TH BIRTHDAY (INVITED ONLY)</u>	
Adiabatic Motion and Statistical Mechanics Via Mass-Zero Constrained Dynamics	83
<i>Giovanni Cicotti</i>	
383a Computational Design of Peptides as Biomarkers, Sensors, Detectors and Drugs.....	84
<i>Carol Hall</i>	
383c Capillary Condensation and Hysteresis in Nanoporous Materials: New Simulations and New Insights	85
<i>Zhao Li, Randall Snurr</i>	
383d Robust Phase Equilibria in Reactive Non-Ionic and Ionic Systems Relevant to Pharmaceutical Applications.....	86
<i>Amparo Galindo</i>	
383e Charting the Design Space of Chemically-Heterogeneous Surfaces that Manipulate Water-Mediated Interactions	87
<i>M. Scott Shell</i>	
383f Wetting and Electrowetting of Polyelectrolyte Complex Coacervates on Solid Surfaces.....	88
<i>Christopher Balzer, Pengfei Zhang, Zhen-Gang Wang</i>	
383g Free Energy Barriers for Anti-Freeze Protein Engulfment: a Model for the Effects of Supercooling, Footprint Size, and Neighbor Distances	89
<i>Hossam Farag, Baron Peters</i>	
<u>PLENARY SESSION: COMPUTATIONAL MOLECULAR SCIENCE AND ENGINEERING FORUM (INVITED TALKS)</u>	
541a Understanding and Controlling Properties of Biomimetic Polymers.....	90
<i>Jim Pfaendtner</i>	
541b the Influence of Halides on the Solution-Phase Growth of Cu Nanowires and Microplates: a Multi-Scale Theoretical Study.....	91
<i>Kristen Fichthorn</i>	
541c Mechanochemical Activation in Nanostructured Triblock Copolymers: a Computational Study	92
<i>Antonia Statt</i>	
541d Modeling the Recycling of Polymer Waste	93
<i>Sanat K. Kumar</i>	
541e How Molecular Simulations Are Being Used to Phase Out High Global Warming Potential Hydrofluorocarbon Refrigerants.....	94
<i>Edward Maginn</i>	

PRACTICAL APPLICATIONS OF COMPUTATIONAL CHEMISTRY AND MOLECULAR SIMULATION FOR COMPLEX FLUIDS AND PHASE BEHAVIOR

431a A Quantitative, Molecular Simulations Based, Kinetic Model of Acid Gas Absorption in Aqueous Amines.....	95
<i>Frederick De Meyer, Bénédicte Poulaïn, Xavier Rozanska</i>	
431b Accessible DPD Models for Structured Formulations Via Automated and Atomistically-Driven Parameterization.....	96
<i>David A. Nicholson, John C. Shelley, Andrea Browning, Mayank Misra, Mohammad Atif Faiz Afzal, Paulo G. M. Mileo, H. Shaun Kwak, Mathew D. Halls</i>	
431c Multi-Scale Simulations Relevant for Hydrates Management.....	97
<i>Alberto Striolo, Alberto Striolo</i>	
431d Progress Towards Alchemical Simulations Driven by Many-Body Gradient-Domain Machine Learning	98
<i>Alex M. Maldonado, John Keith</i>	
431e Exploration of the Retention Mechanism in Supercritical Fluid Chromatography by Molecular Simulations.....	99
<i>Chun-Kai Chang, Joern Siepmann, Faith L. Wroniuk, Yih Ling Saw, James P. Grinias, Mark R. Schure, Stephanie A. Schuster</i>	
431f Impacts of Surface Functionalization on the Cellulose Nanocrystal Solubility in Ethanol.....	100
<i>Arash Elahi, Santanu Chaudhuri</i>	
431g Rational Design of Solvents for Catalytic Transformation of Biorenewable Platform Chemicals	101
<i>Mohd Ussama, Gourav Shrivastav, M. Ali Haider</i>	

RECENT ADVANCES IN MOLECULAR SIMULATION METHODS

103a Brownian Bridges for Stochastic Chemical Processes – Applications and Approximation Method	103
<i>Vivek Narsimhan, Shiyang Wang, Anirudh Venkatesh, Doraiswami Ramkrishna</i>	
103b Supervised Learning and the Finite-Temperature String Method for Computing Commitor Functions and Reaction Rates.....	104
<i>Muhammad Hasyim, Clay Batton, Kranthi K. Mandadapu</i>	
103d Systematic Control of Collective Variables Learned from Variational Autoencoders	105
<i>Jacob I. Monroe, Vincent K. Shen</i>	
103e Accelerated Free Energy Calculations by Joint Biasing in Configurational and Alchemical Space in Metadynamics	106
<i>Wei-Tse Hsu, Pascal Merz, Giovanni Bussi, Michael Shirts</i>	
103f Exploring Low-Energy Regions of Glassy Potential Energy Landscapes.....	107
<i>Amruthesh Thirumalaiswamy, Robert Riggleman, John C. Crocker</i>	
103g Ordinary Least Squares, Extraordinary Overconfidence: Towards Improved Statistical Estimators for Particle Diffusivity.....	108
<i>Kevin S. Silmore, Yuanhao Li, Gerald J. Wang</i>	

103h How to Quantify Spatial Variations in Diffusivity in Molecular Dynamics Simulations.....	109
<i>Tiago Domingues, Ronald Coifman, Amir Haji-Akbari</i>	
103i Leveraging the Wolf Method for Electrostatics to Extend Time and Length Scales Accessible by Monte Carlo Simulations.....	110
<i>Gregory Schwing, Mohammad Soroush Barhaghi, Brad Crawford, Loren Schwiebert, Jeffrey Potoff</i>	
103j py-MCMD: Hybrid Monte Carlo – Molecular Dynamics Simulations.....	112
<i>Brad Crawford, Mohammad Soroush Barhaghi, Gregory Schwing, David Hardy, John Stone, Loren Schwiebert, Jeffrey Potoff, Emad Tajkhorshid</i>	

RECENT ADVANCES IN MULTISCALE METHODOLOGIES

233a Symmetric Molecular Dynamics	114
<i>Andrew White</i>	
233b an Extended-Ensemble Relative Entropy Approach to Sequence-Specific Coarse-Grained Models for Peptide Aggregation.....	115
<i>Evan Pretti, M. Scott Shell</i>	
233c Drl Take the Wheel: Employing Deep Reinforcement Learning to Drive Vaccine Models.....	116
<i>Jonathan Faris, Daniel Orbidan, Brenden Petersen, Kayla Sprenger</i>	
233d Accelerated Kinetic Monte Carlo (kMC) Simulation and Density Functional Theory (DFT) to Predict Turn-Over Frequencies in Heterogeneous Complex Catalytic Reactions	117
<i>Silabrata Pahari, Chi-Ho Lee, Joseph Kwon</i>	
233e Towards the Elimination of Backmapping in Multiscale Simulations	119
<i>Nicholas Jackson</i>	
233f Implicit Heuristic Model Captures Electrostatic Features of Cell Membrane Environment.....	120
<i>Rituparna Samanta, Jeffrey J. Gray</i>	
233g Hamiltonian-Resolution Replica Exchange Improves Flexible Backbone Protein Docking by Mimicking Induced-Fit Pathways	121
<i>Ameya Harmalkar, Jeffrey J. Gray</i>	
233h Modeling the Influence of Glycosylation on Protein Interaction	122
<i>Bradley Harris, Yihan Huang, Zachary Rollins, Karen A. McDonald, Somen Nandi, Priya Shah, Steven George, Roland Faller</i>	
233i Multiscale Molecular Modeling of Flory-Huggins χ -Parameter Calculation and Simulation of Structural Transformation of Photo-Regulated Multicompartment Micelle	123
<i>Jinwon Cho, Ji Il Choi, Seung Soon Jang</i>	

SOFTWARE ENGINEERING IN AND FOR THE MOLECULAR SCIENCES

687a VACUUMMS: Stewardship of Research Software from the Void.....	124
<i>Frank Willmore</i>	
687b Polymerizeit! Software to Generate Molecular Structures of Crosslinked Polymers in Silico.....	125
<i>Salman Bin Kashif, Sapna Sarupria</i>	

687c Validating a New Force Field and Extensible Analysis for a Large-Scale Screening Study of P3HT	126
<i>Jenny Fothergill, Eric Jankowski</i>	
687d MoSDeF-GOMC: Python Software for The creation of Scientific Workflows for the Monte Carlo Simulation Engine GOMC	127
<i>Brad Crawford, Umesh Timalsina, Co Quach, Nicholas C. Craven, Justin Gilmer, Peter Cummings, Jeffrey Potoff</i>	
687e Chempred: Machine Learning for Molecular Property Prediction	129
<i>Charles McGill, Esther Heid, Yunsie Chung, Kevin Greenman, David Graff, Mengjie Liu, Camille Bilodeau, Rafael Gomez-Bombarelli, Connor Coley, Klavs Jensen, Tommi S. Jaakkola, Regina Barzilay, William Green</i>	
687f Workflow Automation in Predicting Exciplex Formation in Arene-Amine Complexes	130
<i>Abhilash Patra, Shaama Mallikarjun Sharada</i>	

687g Parallelization of Grand Canonical Ensemble Monte Carlo Using Prefetching and Windowing of Flat Histogram Simulations.....	131
<i>Harold Hatch, Vincent K. Shen</i>	

687h Pscf+: an Extended and Improved Open-Source Software Package for Polymer Self-Consistent Field Calculations of Block Copolymer Self-Assembly	132
<i>Juntong He, Qiang Wang</i>	

SPOTLIGHTS IN THERMODYNAMICS AND COMPUTATIONAL MOLECULAR SCIENCE (INVITED TALKS)

297a Embedding Stereoelectronic Effects into Molecular Representations for Machine Learning	133
<i>Gabe Gomes</i>	

297b Predicting Solubility Limits of Organic Solutes for a Wide Range of Solvents and Temperatures Using Machine Learning and Thermodynamics	134
<i>Florence Vermeire, Yunsie Chung, William Green</i>	

297c Towards a Universal Adsorption Model Using Machine Learning: Motivation, Progress and Challenges	137
<i>Diego Gomez Gualdrón</i>	

297d Atomistic Simulations of RNA Folding in Bulk Aqueous Solutions and Under Confinement.....	138
<i>Gul Zerze</i>	

Effect of Free Volume Elements on the Local Dynamics of Glassy Polymers from Molecular Dynamics Simulations.....	139
<i>Janani Sampath</i>	

297e Thermodynamic Stability of Multimetallic Nanoparticles.....	140
<i>Giannis Mpourmpakis</i>	

297f Probing Realistic Water-2D Material Interfaces Via Combined Quantum and Classical Simulations.....	141
<i>Ananth Govind Rajan</i>	

THE INDUSTRIAL FLUID PROPERTIES SIMULATION CHALLENGE

711A Correlating and Predicting Thermodynamic Properties of Fluid Mixtures in Phase Equilibrium and Adsorption Equilibria	142
<i>Chau-Chyun Chen</i>	
711B Machine Learning for Predicting the Viscosity of Binary Liquid Mixtures.....	143
<i>Camille Bilodeau, Andrei Kazakov, Sukrit Mukhopadhyay, Jillian Emerson, Tom Kalantar, Chris Muzny, Regina Barzilay, Klavs Jensen</i>	
711C Computational Evaluation of Liquid Mixtures Using Physics-Based Models and Machine Learning	144
<i>Mohammad Atif Faiz Afzal, Garvit Agarwal, Andrea Browning, Mathew D. Halls</i>	
711D Predicting Properties of Ionic Liquid Mixtures Using Molecular Simulations and Machine Learning	145
<i>Jindal Shah</i>	
711E A Multi-Scale Computational Framework for Property Prediction of Fluid Mixtures.....	146
<i>Marianna Yiannourakou, Xavier Rozanska, Benoit Minisini</i>	

APPLICATIONS OF MOLECULAR MODELING TO STUDY INTERFACIAL PHENOMENA II

46a Characteristics of Droplet Explosions Studied with Non-Equilibrium Molecular Dynamics Simulations	147
<i>Dominik Schaefer, Babette Kunstmann, Maximilian Kohns, Hans Hasse</i>	
46b Bubble Nucleation in the Surfactant Stabilized Polyol-CO ₂ Mixtures: Insights from a Classical Density Function Theory Study	148
<i>Sriteja Mantha, Huikuan Chao, Andrew Ylitalo, Benjamin Laccetti, Thomas Fitzgibbons, Weijun Zhou, Valeriy Ginzburg, Richard C. Flagan, Julia A. Kornfield, Zhen-Gang Wang</i>	
46c Interfacial Thermodynamics of Cryogenic Fluids: the Effect of Non-Condensable Gas on Fluid Storage.....	149
<i>Michael Delyser, Ashwin Ravichandran, Wayne J. Mullinax, John W. Lawson</i>	
46d Energy Optimization of Nanochannel Fluid Extraction with Various Channel Geometries	150
<i>Zachary Diermyer, Yidong Xia, Jiaoyan Li</i>	
46f Free-Energy of Monomeric Species in Uio-66 Metal-Organic Framework	151
<i>Sanoj, Yamil Colón</i>	
46g Structural Origin of Multiple Alkylated Cyclopentane as an Effective Lubricant.....	152
<i>Jee-Ching Wang, Vudit Singh</i>	
46h Extracting Anisotropy Strength and Interfacial Free Energy of Al-Mg Alloy Under Rapidcooling Conditions Using Molecular Dynamics Simulations	153
<i>Daniel Dolce, Pabitra Choudhury</i>	
46i Dynamic Evolution of Atomically Dispersed Catalysts	154
<i>Nicholas Humphrey, Selin Bac, Shaama Mallikarjun Sharada</i>	
46j Molecular Simulations Study of Calcium Carbonate-Amino Acid-Dentin Interactions.....	155
<i>Alina Emelianova, Max Maximov, Tatiana V. Brinzari, Andrei Potanin, Gennady Gor</i>	

MACHINE LEARNING FOR SOFT MATERIALS II

656a A New Computational-Experimental Screening Methodology Identifies More Effective Solvents for CO ₂ Capture	156
<i>Frederick De Meyer, Alexey Orlov, Christophe Coquelet, Xavier Rozanska</i>	
656b Characterization of Chemoresponsive Liquid Crystals Using Topological Descriptors and Machine Learning.....	157
<i>Shengli Jiang, Nanqi Bao, Alexander Smith, Nicholas L. Abbott, Victor Zavala</i>	
656c Physics-Informed Deep Neural Networks for Predicting Fluid Flow in Complex Porous Materials.....	159
<i>Serveh Kamrava, Muhammad Sahimi</i>	
656d Simulation of Neutron Dark Field Interferometry Data in Hierarchical Materials Using Small Angle Scattering Models	160
<i>Caitlyn Wolf, Youngju Kim, Anis Ben Said, Sarah Robinson, Ryan P. Murphy, M. Cyrus Daugherty, Michael Huber, David L. Jacobson, Jacob Lamanna, Nikolai Klimov, Paul Kienzle, Peter Bajcsy, Daniel S. Hussey, Katie Weigandt</i>	
656e Developing an ML Algorithm to Predict the Aqueous Solubility of Polymers and Organic Compounds.....	161
<i>Arash Tayyebi, Ali Alshami</i>	
656g Machine Learning for the Discovery of Molecular Recognition Based on Single-Walled Carbon Nanotube Corona-Phases.....	162
<i>Xun Gong, Nicholas J Renegar, Retsef Levi, Michael Strano</i>	
656h Accelerated Discovery of Novel Ionic Liquid Cations Using a Continuous Latent Space Representation of Chemical Space	163
<i>Pratik Dhakal, Jindal Shah</i>	
656i Context-Aware Representations from Deep Learning for Antibody Design	164
<i>Sai Pooja Mahajan, Jeffrey J. Gray</i>	

PRACTICAL APPLICATIONS OF COMPUTATIONAL CHEMISTRY AND MOLECULAR SIMULATION FOR SOLVENTS AND INORGANIC MATERIALS

482a Mechanochemical Degradation Pathways of Protective Oxide Surfaces: Development of an Ab-Initio Informed Multiscale Corrosion Model	165
<i>Jeremy Scher, Tae Wook Heo, Yue Hao, Matthew Kroonblawd</i>	
482b Molecular Insights into NMR Relaxation of Gd(III)-Based Contrast Agents for MRI Applications.....	166
<i>Thiago Jose Pinheiro Dos Santos, Arjun Valiya Parambathu, Dilip Asthagiri, Philip Singer, Walter Chapman</i>	
482c Interface Force-Field (IFF) Parameterization of Ti ₃ C ₂ T _x MXenes	167
<i>Isaac Armstrong, Vikas Varshney, Hendrik Heinz</i>	
482d Molecular Characterization of High Ionic Conductivity in Fluoroether Lithium Metal Battery Electrolytes.....	168
<i>Yuxi Chen, Elizabeth Lee, Juan J. De Pablo</i>	

482e Ab Initio Study on the Reaction Kinetics of Ethylene Glycol Decomposition on Pt (111) and Pt ₃ Sc (111).....	169
<i>Shedrack G. Akpe, Hyung Chul Ham</i>	
482f Oxidation Rate and Leaching of Flame-Made Nanosilver by Reactive Molecular Dynamics.....	171
<i>Eirini Goudeli, Diego Chaparro</i>	
482g Molecular Dynamic Insights on the Distinct Solvation Structures of Aromatic and Aliphatic Compounds in Monoethanolamine Based Deep Eutectic Solvents.....	172
<i>Nikhil Kumar, Tamal Banerjee</i>	

RECENT ADVANCES IN MOLECULAR MODELING OF INTERFACIAL THERMODYNAMICS AND DYNAMICS

181a Optiboost: a Method for Choosing a Safe and Efficient Boost for the Bond-Boost Method in Accelerated Molecular Dynamics Simulations with Hyperdynamics	173
<i>Jianming Cui, Kristen Fischhorn</i>	
181b Coupling Replica Exchange with Backbone Sampling Captures Conformational Changes on Protein-Protein Interfaces.....	174
<i>Ameya Harmalkar, Jeffrey J. Gray</i>	
181c Molecular Modes from NMR Relaxation in Fluids: Going Beyond the Bpp Theory	175
<i>Arjun Valiya Parambathu, Philip Singer, Thiago Jose Pinheiro Dos Santos, George J. Hirasaki, Walter Chapman, Dilip Asthagiri</i>	
181d Unbiased Coarse-Grained Monte Carlo Simulation Using SAXS-Data for Identification of Self-Assembled Nanostructures	176
<i>Silabrata Pahari, Shuhao Liu, Mustafa Akbulut, Joseph Kwon</i>	
181e Equilibrium Adsorption Morphologies of Surfactants at Metal-Water Interfaces Studied Using a Novel Free Energy Sampling Methodology in Molecular Simulations	178
<i>Sumit Sharma, Himanshu Singh</i>	
181f a Molecular Dynamics Simulation Study of the Kapitza Heat Transfer Resistance.....	179
<i>Sebastian Schmitt, Simon Stephan, Hans Hasse</i>	
181g Molecular Modeling of Alcohol Effects in Nonionic Surfactant Micelles with Density Functional Theory	180
<i>Jinxin Lu, Walter Chapman</i>	
181h Extracting Solid-Melt Interfacial Free Energy and Anisotropy Strength of Al-Cu Alloy Using Molecular Dynamics Simulations	181
<i>Amrutduty Swamy, Pabitra Choudhury, Daniel Dolce</i>	
181i Molecular Dynamics Simulation of O ₂ Transport in Nafion.....	183
<i>Nicholas Tiwari</i>	
181j Coarse-Grained Molecular Dynamics Investigation of Adsorption of Type IV Pili Proteins onto Graphene-Cu(111) and Defective Graphene-Cu(111) Interfaces.....	184
<i>Sourav Verma, Marina Davidson, Kenneth Benjamin</i>	

PRACTICAL APPLICATIONS OF COMPUTATIONAL CHEMISTRY AND MOLECULAR SIMULATION FOR POLYMERS AND BIOLOGICAL SYSTEMS

585a Structure Enumeration Algorithm for Silicone Mq-Resins.....	185
<i>Steven G. Arturo, Thomas D. Bekemeier, Don Eldred, Wei Gao, James H. Wade, Tianlan Zhang</i>	
585c Force Fields for the Prediction of Transport Properties of Lubricants at Extreme Conditions	186
<i>Sebastian Schmitt, Simon Stephan, Hans Hasse</i>	
585d Understanding Electronic Properties of 1-N-Alkyl-3-Methylimidazolium Chloride Ionic Liquids with Iron Porphyrin	187
<i>Sudip Kumar Das, Jindal Shah</i>	
585e Applying Deep Learning to Accelerate Molecular Dynamics Simulation-Based Structural Properties Prediction for Biomolecules.	188
<i>Pin-Kuang Lai</i>	
585f Comparison of Dissociation Kinetics and Mechanism of Classical and Non-Classical Cannabinoids from Cannabinoid Receptors	189
<i>Soumajit Dutta, Diwakar Shukla</i>	
585g Indacenodinaphthothiophene Isomers with Polyradical Character.....	190
<i>Md Abdus Sabuj, Md Masrul Huda, Chinmoy Saha, Neeraj Rai</i>	

Author Index