

Computational Molecular Science and Engineering Forum 2016

Core Programming Area at the 2016 AIChE Annual Meeting

San Francisco, California, USA
13 - 18 November 2016

ISBN: 978-1-5108-3431-6

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© (2016) by AIChE
All rights reserved.

Printed by Curran Associates, Inc. (2017)

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

(7t) Accelerating Materials Design: Computer Simulations and QSAR Modeling	1
<i>Qing Shao</i>	
(7u) Computationally Assisted Discovery of Well-Designed Materials for Applications to Energy, Environment, and Catalysis	2
<i>Ki Chul Kim</i>	
(7w) Computationally Driven Discovery of Novel Materials for Separation and Catalysis	3
<i>Peng Bai</i>	
(7b) Towards Accurate Atomistic Description of Reactive Interfaces for in silico Design of Novel Functional Materials	4
<i>Badri Narayanan</i>	
(7c) Solubility and Thermodynamic Properties of α-Amino Acids in a Model System of Industrial Residues	7
<i>Nathan Bowden</i>	
(7r) Dispersion-Corrected Density Functional Tightening Binding Modeling of the Natural Metastable Twin Boundary of Organic Energetic Materials: Beta-Octahydro-1,3,5,7-Tetranitro-1,3,5,7-Tetrazocine	8
<i>Zhichao Liu, Weuhua Zhu</i>	
(7v) Quantitatively Reliable Molecular Modeling and Simulation of Vapor-Liquid Equilibria	9
<i>Martin Horsch, Stephan Werth, Katrin Stöbener, Hans Hasse</i>	
(7h) Modeling Chemical Reactivity for Nanoscale Design	11
<i>Ryan Gotchy Mullen</i>	
(7i) Enhanced Molecular Simulations for Applications in Protein Stabilization, Crystallization, and Structural Determination	12
<i>Vance Jaeger</i>	
(7j) Advanced Materials Design Using Molecular Simulation, Evolutionary Computing and Machine Learning	15
<i>Tarak Kumar Patra</i>	
(7d) Exploring Fundamentals of Zeolite Catalysis – A Theoretical Perspective	16
<i>Florian Göttl</i>	
(7e) Reverse Engineering of Molecular Structure	18
<i>Farhad Gharagheizi</i>	
(7f) Developing Molecular Theories/Simulations to Understand and Optimize Soft Matter Systems: From Ions to Polymers to Gels	19
<i>Rui Wang</i>	
(7g) Simulation of Selectively Permeable Novel Polymeric Membranes	20
<i>Marielle Soniat</i>	
(7p) Towards More Rational Design of Electrocatalyst for Carbon Dioxide Reduction	21
<i>Jianping Xiao, Jens Norskov, Karen Chen</i>	
(7k) Computational Soft Matter	22
<i>Jens Glaser</i>	
(7l) Design and Discovery of Multifunctional Nanoporous Materials	23
<i>Ambarish R. Kulkarni</i>	
(7m) Hydrodynamic Model of Complex Liquids with Microstructure	24
<i>Rui Zhang</i>	
(7q) New Generation of Polarizable Reactive Force Fields for Multiscale Simulations of Complex Materials	26
<i>Saber Naserifar</i>	
(7x) Flexible and Dynamic Porous Crystals	29
<i>Cory Simon</i>	
(7n) Computational and Experimental Investigation of Membrane Biomechanics	30
<i>Manuela A.A. Ayee</i>	
(7o) Machine Learning and Molecular Dynamics Map Conformational Landscape of μ-Opioid Receptor	31
<i>Amir Barati Farimani, Evan N. Feinberg</i>	
(51d) Monte Carlo Molecular Simulations of Water/Oil Interfacial Tension at Elevated Temperatures and Pressures	32
<i>Jingyi Chen, Bai Xue, David B. Harwood, Qile Chen, J. Ilja Siepmann</i>	
(51e) Interfacial Tension Prediction of Water/Oil Mixtures Using Stabilized Density Gradient Theory and Using iSAFT Density Functional Theory	33
<i>Xiaoqun Mu, Le Wang, Amin Haghmoradi, Walter G. Chapman</i>	
(51f) Prediction of the Water/Oil Interfacial Tension from Molecular Simulations Using the Coarse Grained SAFT-γ Mie Force Field	34
<i>Carmelo Herdes, Åsmund Ervik, Andres Mejía, Erich A. Müller</i>	
(51g) Industrial Fluid Properties Simulation Collective 9th Challenge	35
<i>Konstantinos D. Papavasileiou, Othonas A. Moulτος, Ioannis G. Economou</i>	
(62a) Molecular Dynamics Study of Surfactant and Oil Interactions at Saltwater-Air Interfaces	36
<i>Leebyn Chong, Yungchieh Lai, Fan Shi, McMahan L. Gray, Yee Soong, Yuhua Duan</i>	
(62b) Molecular-Scale Description of SPAN80 Desorption from the Squalane-Water Interface	37
<i>Liang Tan, Lawrence R. Pratt, Mangesh Chaudhari</i>	

(62c) Some Effects of Surface Heterogeneity on the Morphology of Surfactant Self-Assembled Aggregates	43
<i>Alberto Striolo</i>	
(62d) Adsorption of Surfactants on Metallic Surfaces Studied Using Molecular Simulations	44
<i>Sumit Sharma</i>	
(62f) Quantum Chemistry Study of Curvature Effects on Boron Nitride Nanotube/Nanosheet for Gas Adsorption	45
<i>Haoyan Sha, Roland Faller</i>	
(62g) Molecular Simulation of Metal-Ionic Liquid Interfaces	46
<i>Matt Thompson, Peter T. Cummings, Robert Sacci, Jennifer Black, Nina Balke</i>	
(62h) Effects of Fluoroethylene Carbonate and Dissolved Manganese on the ANODE SEI Layer Using Reaxff-Based Molecular Dynamics	47
<i>Sahithya Reddivari, Christian Lastoskie</i>	
(62i) Formation Mechanisms for Microscopic Precursors in Droplet Spreading	48
<i>Rolf E. Isele-Holder, Ahmed E. Ismail</i>	
(142a) Mathematics for Data-Driven Modeling - The Science of Crystal Balls	49
<i>Ioannis G. Kevrekidis</i>	
(142b) Decoding Common Features of Protein-Nanoparticle Interactions	50
<i>Qing Shao, Carol K. Hall</i>	
(142c) Design of Optimal Experimental Probes for Protein Dynamics Using Machine Learning and Variational Approach to Modeling Conformational Kinetics	51
<i>Balaji Selvam, Shriyaa Mittal, Chuankai Zhao, Diwakar Shukla</i>	
(142d) Guiding Experiments Towards New Functional Materials with Informatics	52
<i>Prasanna V. Balachandran, Dezhen Xue, Turab Lookman</i>	
(142e) Pushing the Frontiers of Atomistic Modeling Towards Predictive Design of Materials.....	53
<i>Subramanian Sankaranarayanan, Badri Narayanan, Mathew Cherukara</i>	
(142f) Design of Ternary Transparent Conducting Oxides	54
<i>Christopher Sutton, Matthias Scheffler, Luca M. Ghiringhelli</i>	
(142g) Development of Empirical Charge Transfer Interatomic Potential for Tantalum Oxide Nanostructures from First Principle Calculations	55
<i>Kiran Sasikumar, Badri Narayanan, Subramanian K.R.S. Sankaranarayanan</i>	
(142h) Machine Learning for Advancing Discovery of Novel Thermoelectric Materials. The Thermoel.....	56
<i>Al'ona Furmanchuk, Ankit Agrawal, James Saal, Jeff Doak, Gregory Olson, Alok Choudhary</i>	
(142i) Identifying Descriptors for Dielectric Breakdown Strength Using Genetic Programming	57
<i>Fenglin Yuan, Tim Mueller</i>	
(142j) Machine Learning with Structural Fingerprints of Local Particle Environments	58
<i>Matthew Spellings, Sharon C. Glotzer</i>	
(142k) Using Semi-Supervised Machine Learning to Map the Phase Diagrams of Open Materials Data Sets	59
<i>Jason Hattrick-Simpers, Jonathan Kenneth Bunn, Jianjun Hu</i>	
(156a) The Prediction of Environmentally Important Properties for Hazardous Chemicals	60
<i>Stanley Sandler</i>	
(156b) Corresponding States Theory for Property Prediction at the Nanoscale.....	61
<i>Keith E Gubbins</i>	
(156c) Heat Induced and UV Induced Grafting of Poly(glycidyl methacrylate) on PBT Nonwovens for Bioseparations	62
<i>Ruben G. Carbonell, Michael Heller, Benham Pourdeyhimi</i>	
(156d) Thermodynamics and Statistical Mechanics of Drying at the Nano-Scale	63
<i>Pablo G. Debenedetti, Y. Elia Altabet</i>	
(156e) Harmonically-Mapped Averaging Applied to Lennard-Jones Crystal Phase	64
<i>Andrew J. Schultz, Apoorva Purohit, David A. Kofke</i>	
(156f) Computational-Hydrodynamic Studies of the Noh Compressible Flow Problem Using Non-Ideal Equations of State	65
<i>Kevin Honnell, Sarah Burnett, Scott Ramsey</i>	
(156g) Lattice Models, Polymers and DNA Topology	66
<i>Chris Soteris</i>	
(156h) Design of Macromolecular Biomaterials Using Atomistic and Coarse-Grained Molecular Simulations.....	67
<i>Arthi Jayaraman, Ahmadreza F. Ghobadi</i>	
(156i) Rational Design of Peptide-Based Stimuli-Responsive Biomaterials Via Multiscale Modeling	68
<i>Hung D. Nguyen</i>	
(196a) Altsep: Sustainable Separation Processes Roadmap Review.....	69
<i>Robert Giraud, Glenn Lipscomb</i>	
(220a) Slip Slidin' Away: Three Decades of Adventures in Computational Rheology and Lubrication	70
<i>Peter T. Cummings, Clare McCabe, Christoph Klein, Christopher R. Iacovella</i>	
(220b) How to Make Particles Interact in Multiple Directions and Form Interconnected Networks: Colloidal Assembly Based on Field-Induced Multipoles.....	71
<i>Orlin D. Velev, Bhuvnesh Bharti</i>	
(220c) Polymers in Ionic Liquids	72
<i>Arun Yethiraj</i>	
(220d) Collective Dynamics of Dipolar and Multipolar Colloids: From Passive to Active Systems	73
<i>Sabine H.L. Klapp</i>	

(220e) Promising Vistas for Applied Chemical Thermodynamics: Statistical Mechanics As a First Step Toward Thermodynamic Properties	74
<i>John Prausnitz</i>	
(220f) A Biased Review about Computer Simulations of Protein Folding and Aggregation	75
<i>Daniel Forciniti</i>	
(220g) “Grafting through” Polymerization	76
<i>Jan Genzer</i>	
(220h) Understanding Temperature-Responsive Behavior of Elastin-like Polypeptides	77
<i>Yaroslava G. Yingling</i>	
(220i) Utilizing Multivariate Analysis to Enhance Bioprocess Development and Operation	78
<i>Mauricio Futran</i>	
(220j) Self-Assembly of Colloids in Ordered Carrier Fluids	79
<i>Martin Schoen</i>	
(253k) Role of Van Der Waals and Entropy on Gold Cluster (meta)Stability	80
<i>Bryan R Goldsmith, André Fielicke, Matthias Scheffler, Luca M. Ghiringhelli</i>	
(253b) Simulating NMR Relaxation Time Constants of Benzene in MOF-5 to Investigate Phase Coexistence	81
<i>Efrem D. Braun, Sondre K. Schnell, Jeffrey A. Reimer, Berend Smit</i>	
(253bm) Supramolecular Polymer Hydrogel Design through Molecular Dynamics Study of Octa-Acid Cavitand and Adamantane	82
<i>A. L. Saltzman, Hank Ashbaugh</i>	
(253a) Resolving Experimentally-Inferred Solvophobic Interactions in the Overlap Region	83
<i>J. Wesley Barnett, Amna Bhutta, Sarah Bierbrier, Natalia da Silva Moura, Hank Ashbaugh</i>	
(253aa) Computation of Chemical Potential of Water at Low Temperatures	84
<i>Ali Poursaeidesfahani, Ahmadreza Rahbari, David Dubbeldam, Thijs Vlugt</i>	
(253y) Multi-Scale Coarse Graining of Polarizable Models Through Force-Matched Dipole Fluctuations	85
<i>Patrick G. Lafond, Sergei Izvekov, Jan W. Andzelm, Timothy W. Sirk</i>	
(253ac) Desolvation Barriers in Ionic Crystal Growth	86
<i>Mark Joswiak, Michael F. Doherty, Baron Peters</i>	
(253ah) Mechanism of the Fcc-Hcp Phase Transformation in Solid Ar	87
<i>Bingxi Li, Roland Faller</i>	
(253bz) Prediction of the Sooting Tendencies of Candidate Biofuels from Molecular Structure Via an Artificial Neural Network	88
<i>Peter St. John, Drubajyoti Das, Charles S. McEnally, Lisa D. Pfefferle, Yannick J. Bomble, Seonah Kim</i>	
(253c) Radical Mechanism for Low Temperature C-O Bond Activation on Metal/Metal Oxide Catalysts	89
<i>Alexander V. Mironenko, Dionisios G. Vlachos</i>	
(253d) Understanding Unfolded and Intrinsically Disordered Proteins Via Molecular Simulations	90
<i>Gul H. Zerze, Jeetain Mittal</i>	
(253f) Understanding the Shape-Control Mechanism in the Solution-Phase Growth of Ag Nanocrystals	91
<i>Tonnam Balankura, Kristen Fichthorn</i>	
(253ae) Extraction of Pairwise Interaction Potentials from Cohesive Energy Inversions—a General Approach with DFT	92
<i>Victor R. Vasquez, Kevin Schmidt</i>	
(253g) Molecular Dynamics of Inorganic and Organic Interfaces, Parametrization Based on Quantum Mechanical Simulation	93
<i>Hiroya Nitta, Kosuke Ohata, Kenta Chaki, Taku Ozawa</i>	
(253e) Kinetic Analysis for Molecular Simulations of Nucleation Processes with Low Barriers	94
<i>David A. Nicholson, Gregory C. Rutledge</i>	
(253h) First-Principles Density Functional Theory Modeling Assisted Understanding on the Redox Properties of Nitrogen Doped Organic Molecules	95
<i>Jiwoong Kang, Seung Soon Jang, Ki Chul Kim</i>	
(253bx) Automated Spatial Analysis of NFκB in Multispectral Images of Cerebrovascular Endothelial Cells	96
<i>Edward P. Gatzke, Kasey Catalfomo, Melissa A. Moss, Lauren Wolf</i>	
(253i) A Grand Canonical Monte Carlo Simulation-Based Method for the Calculation of Electrical Potential Inside Nano-Porous Electrodes	97
<i>Patricia Taboada-Serrano, Evan Ney</i>	
(253bw) Meta-Analysis of Cellular Toxicity of Cadmium-Containing Quantum Dots Using Bayesian Networks	98
<i>Muhammad Bilal, Rong Liu, Eunkeu Oh, Igor Medintz, Yoram Cohen</i>	
(253ak) Effects of Self-Energy of the Ions on the Double Layer Structure and Properties at the Dielectric Interface	99
<i>Rui Wang, Zhen-Gang Wang</i>	
(253bo) Predicting Protein Dynamics in Complex Environments	100
<i>Vincent Ustach, Roland Faller</i>	
(253r) Automating Workflows for Surface Science and Catalysis	101
<i>Joseph H. Montoya, Kristin Persson</i>	
(253s) Potential of Mean Force of siRNA and Pmal: Molecular Dynamics and Theoretical Analysis	102
<i>Jipeng Li, Diannan Lu, Jianzhong Wu</i>	
(253l) First Principles Computational Study on Adsorption of Organic Methyl Iodide in Triethylenediamine Impregnated Activated Carbon	103
<i>Byungchan Han, Hoje Chun</i>	

(253p) Evaluation of Effective Stacking Interactions of Kaolinite Nanoparticles in Aqueous and Organic Solvents By Molecular Theory of Solvation	104
<i>Stepan Hlushak, Stanislav R. Stoyanov, Andriy Kovalenko</i>	
(253u) Mapped Averaging for Highly Efficient Evaluation of Fluid-Phase Properties By Molecular Simulation	105
<i>Weisong Lin, Akshara Goyal, Andrew J. Schultz, David A. Kofke</i>	
(253x) Molecular Dynamics Simulation of Cations (K+, Na+, Rb+, Mg2+ and Sr2+) Adsorption at the Muscovite Mica - Aqueous Solution Interface	106
<i>Sai Krishna Reddy Adapa, Ateeque Malani</i>	
(253br) Understanding the Influence of Curcumin on Amyloid-β Aggregation at the Molecular Scale	107
<i>Tye D. Martin, David G. Whitten, Eva Y. Chi, Deborah G. Evans</i>	
(253z) Computational Search for Magnetic Nanoparticles to Eradicate Cancer Cells Using the Hyperthermia Approach	108
<i>Shounak Datta, Mario Richard Eden</i>	
(303g) Computational Study of CO2 Adsorption on Apohost and LiCl-Functionalized Zn(bdc)(ted)0.5 Metal-Organic Frameworks	109
<i>Carlos E. Fernandez-Caban, Jorge L. Rosa-Raíces, Paul Meza-Morales, Maria Curet-Arana</i>	
(253v) Practical Data Sharing for Molecular Simulation	110
<i>Jacob R. Boes, John R. Kitchin</i>	
(253bn) Multiscale Simulations of Protein Adsorption on Self-Assembled Monolayers	111
<i>Jian Zhou</i>	
(253ab) Sour Gas Sweetening By Adsorption in Zeolites	112
<i>Mansi S. Shah, Michael Tsapatsis, J. Ilja Siepmann</i>	
(253af) Effects of Ionic Liquids on HP35 Folding Thermodynamics	113
<i>Vance Jaeger, Jim Pfaendtner</i>	
(253al) Sintering of Bimetallic Ag-Au Nanoparticles By Molecular Dynamics	114
<i>Eirini Goudeli, Sotiris E. Pratsinis</i>	
(253bt) Fluid Transport through Nano-Pores: A Stochastic Approach	115
<i>Maria Apostolopoulou, Alberto Striolo, Michail Stamatakis, Richard Day</i>	
(253aq) Structural Changes on Coordination Polymer Ligands (CPL-bpp) Induced By CO2: Theoretical Study Based on Density Functional Theory and Grand Canonical Monte Carlo Simulation	116
<i>Paul Meza-Morales, Maria Curet-Arana</i>	
(253at) Recent Advances in the Development of Cassandra: An Open Source Monte Carlo Framework for Phase Equilibria Calculations	117
<i>Eliseo Marin-Rimoldi, Edward J. Maginn</i>	
(253am) A Transferable Multi-Resolution Coarse-Grained Model for Amorphous Silica Nanoparticles	118
<i>Andrew Z. Summers, Olivia M. Cane, Christopher R. Iacovella, Peter T. Cummings, Clare McCabe</i>	
(253as) Elucidating the Molecular Architecture of the Blood-Brain Barrier Tight Junctions	119
<i>Flaviyan Jerome Irudayanathan, Shikha Nangia</i>	
(253au) Computational Analysis of the Assembly and Catalytic Effects of Self-Assembled Monolayers	120
<i>Gaurav Kumar, Chih-Heng Lien, J. Will Medlin, Michael J. Janik</i>	
(253bp) A Software Ecosystem for the Data-Driven Design of Chemical Systems and the Exploration of Chemical Space	121
<i>Johannes Hachmann</i>	
(253ao) Adaptive Coarse-Graining of Molecular Dynamics through Diffusion Maps	122
<i>David Sroczynski, Anastasia Georgiou, Ioannis G. Kevrekidis, William Gear, Eliodoro Chiavazzo</i>	
(253aw) Molecular Dynamics Simulation of Water and Ion Transport through Carbon Nanotubes	123
<i>Michelle Aranha, Brian J Edwards</i>	
(253ax) Understanding the Structure and Function of Enzymes in ILs for Improved Biocatalysis	124
<i>Kayla Sprenger, Jim Pfaendtner</i>	
(253ay) A General Tool Chain for Screening of Soft Materials	125
<i>Christoph Klein, János Sallai, Trevor J. Jones, Christopher R. Iacovella, Clare McCabe, Peter T. Cummings</i>	
(253o) Integrating Molecular Modelling in Systems Engineering	126
<i>Erich A. Muller, Claire S. Adjiman, George Jackson, Amparo Galindo</i>	
(253m) Evaluating Force Fields Using Wolf2pack's Molecular Database	127
<i>Martin Schenk, Marco Hülsmann, Andreas Krämer, Dirk Reith, Karl N. Kirschner</i>	
(253an) Nusimm: A User-Friendly Cloud Based Web Interface for Performing Molecular Simulations	128
<i>Michael E. Fortunato, Coray M. Colina</i>	
(253bb) Elucidation of Microstructure and Its Connection to Thermophysical Properties of Binary Ionic Liquid Mixtures, a Molecular Simulation Study	129
<i>Utkarsh Kapoor, Jindal K. Shah</i>	
(253bd) A Logic-Based Framework for Defining Force Field Usage Semantics and Atom-Typing Molecular Systems	130
<i>Christoph Klein, Clare McCabe, Peter T. Cummings, János Sallai, Christopher R. Iacovella</i>	
(253bc) Predicting Octanol-Water Partition Coefficient and Force Field Development for NDMA Via Molecular Simulations	131
<i>Himanshu Goel, Shanmuga Venkatesan, Neeraj Rai</i>	
(253be) Exploration of the Hierarchical Roles of Surface Features Facilitating the Adsorption of Biomolecules	132
<i>Wesley Beckner, Jim Pfaendtner</i>	
(253bf) Characterizing Protein Hydration to Inform Its Interactions with Ligands and Other Proteins	133
<i>Erte Xi, Amish Patel</i>	

(253bg) Understanding Wetting-Dewetting Transitions on Nanotextured Surfaces: Implications for Designing Surfaces with Robust Superhydrophobicity	134
<i>Suruchi Fialoke, Erte Xi, Amish Patel</i>	
(253ca) Forming Auxetic Materials from Amorphous Networks	135
<i>Daniel Reid, Nidhi Pashine, Sidney Nagel, Juan De Pablo</i>	
(253ap) Atomistic Picture of the Growth Mechanism of Silicene Monolayers	136
<i>Mathew Cherukara, Badri Narayanan, Ross Harder, Subramanian K.R.S. Sankaranarayanan</i>	
(253q) Sparse Sampling of Water Density Fluctuations	137
<i>Erte Xi, Richard C. Remsing, Suruchi Fialoke, Amish Patel</i>	
(253ar) Hybridization in DNA Self-Assembled Monolayer Studied with Atomistic Simulation and Free Energy Computation	138
<i>Heng Ma, Tao Wei</i>	
(253bj) Development of Transferable Coarse-Grained Force Fields Via Multistate Iterative Boltzmann Inversion	139
<i>Timothy C. Moore, Christopher R. Iacovella, Clare McCabe</i>	
(253bk) Simulation-Based Design of Copolymer Sequence Using the Kinetic Monte Carlo Method	140
<i>Hanyu Gao, Konstantinov Ivan, Steven G. Arturo, Linda J. Broadbelt</i>	
(253cb) Coarse Grained Model of Conformational Disorder Effects on the Electronic States of Poly(3-hexylthiophene) Chains	141
<i>Joel Bombile, Michael Janik, Scott T. Milner</i>	
(304a) Antimicrobial Mechanism of Action of Class IIb Bacteriocins Investigated through Molecular Simulations	142
<i>Panagiota Kyriakou, Yiannis Kaznessis</i>	
(304b) Carbohydrate Recognition Mechanisms in Cellulose-Specific Type B Carbohydrate Binding Modules	143
<i>Abhishek A. Kognole, Christina M. Payne</i>	
(304c) Gold Nanoparticles Change Human Serum Albumin without Denaturing It: A Computer Simulation Study	144
<i>Qing Shao, Carol K. Hall</i>	
(304d) Enhanced Sampling of Protein Structures at the Air-Water Interface	145
<i>Vance Jaeger, Bert de Groot</i>	
(304e) Binding Affinities of Amino Acids on Graphene: Assessment of Force Fields	146
<i>Siva Dasetty, John Barrows, Sapna Sarupria</i>	
(304f) How CO₂ Diffuses into the Active Site of Carbonic Anhydrase: A Study By Molecular Dynamics Simulation and Multi-Scale Markov-State Modeling	147
<i>Gong Chen, Diannan Lu, Jianzhong Wu, Zheng Liu</i>	
(304g) Conformational Ensemble of Islet Amyloid Polypeptide in a Membrane Environment	148
<i>Gregory L. Dignon, Jeetain Mittal, Gül H. Zerze</i>	
(304h) Investigation on the Pathway of Disulfide Bonds Reduction on Human Defensins Using Molecular Dynamics Simulations	149
<i>Liqun Zhang</i>	
(304i) Predicting Protein-Protein Interaction Interfaces, Hot Spots, and Binding Affinities	150
<i>Erte Xi, Amish Patel</i>	
(377a) Best Practices in Collaborative Software Development: Lessons Learned in the Rosetta Commons	151
<i>Jeffrey Gray</i>	
(377b) Validation of Computational Models and Codes	152
<i>Christopher R. Iacovella, Christoph Klein, János Sallai, Ahmed E. Ismail</i>	
(377c) Pysimm: A Python Package for Simulation of Amorphous Polymeric System	153
<i>Michael E. Fortunato, Coray M. Colina</i>	
(377d) Automated Event Detection and Rate Constants for Complex Systems with Reaxff	154
<i>N. Ole Carstensen, Malte Döntgen, Kai Leonhard</i>	
(377e) Freud: A Software Suite for High-Throughput Simulation Analysis	155
<i>Eric S. Harper, Matthew Spellings, Joshua A. Anderson, Sharon C. Glotzer</i>	
(377f) PB-[S]AM, a Novel Solution to the Poisson-Boltzmann Equation for Applications Ranging from Protein Simulations to Polymer Membrane Design	156
<i>Lisa Felberg, Marielle Soniat, David Brookes, Enghui Yap, Teresa Head-Gordon</i>	
(377g) Multi-GPU Electrostatics and Rigid Bodies in HOOMD-Blue 2.0	157
<i>Jens Glaser, Joshua A. Anderson, Sharon C. Glotzer</i>	
(377h) Scientific Data Management with Signac	158
<i>Paul Dodd, Carl Simon Adorf, Sharon C. Glotzer</i>	
(377i) Automated Molecular Modeling Via Optimization of Force Field Parameters	159
<i>Andreas Krämer, Marco Hülsmann, Karl N. Kirschner, Dirk Reith</i>	
(377j) Efficient Neighbor List Calculation for Molecular Simulation of Colloidal Systems Using Graphics Processing Units	160
<i>Michael P. Howard, Joshua A. Anderson, Arash Nikoubashman, Sharon C. Glotzer, Athanassios Z. Panagiotopoulos</i>	
(436a) Methods for Combining Experimental Data and Molecular Simulations into Hybrid Models	161
<i>Andrew White</i>	
(436b) Using Molecular Dynamics to Understand Transmission Electron Microscopy	162
<i>Roland Faller, Nigel D. Browning, Chiwoo Park, David Welch, James E. Evans</i>	
(436c) Pushing the Boundaries of Multiscale Simulation to Model Proton Transport in SERCA	163
<i>Heather B. Mayes, Laura C. Watkins, L. Michel Espinoza-Fonseca, Jessica M. J. Swanson, Gregory A. Voth</i>	
(436d) Modeling the Nucleation of Crystals of Ionic Liquids in the Bulk and Near Graphitic Surfaces	164
<i>Xiaoxia He, Yan Shen, Francisco R. Hung, Erik E. Santiso</i>	

(436e) Improving the Efficiency of Water Adsorption Simulations in Metal-Organic Frameworks	165
<i>Hongda Zhang, Randall Snurr</i>	
(436f) Heterogeneous Ice Nucleation Using Forward Flux Sampling	166
<i>Brittany Glatz, Sapna Sarupria</i>	
(436g) Theoretical Prediction of Interpenetrating Metal-Organic Frameworks	167
<i>Kutay Berk Sezginel, Tianyi Feng, Christopher E. Wilmer</i>	
(436h) First Principles Screening of Transparent Conducting Oxides Using Amobt	171
<i>Alireza Faghaninia, Cynthia S. Lo</i>	
(436i) Polymorphic Transformations at Ambient Conditions Elucidated with Molecular Dynamics	172
<i>Eric Dybeck, Natalie Schieber, Nathan Abraham, Michael R. Shirts</i>	
(436j) NaCl Nucleation from Aqueous Solution By a Seeded Simulation Approach	173
<i>Nils Zimmermann, Bart Vorselaars, David Quigley, Baron Peters</i>	
(478a) Bottom-up Approach to Constructing a Polymerization Process Model: Leveraging New Insights for Improved Manufacturing Performance	174
<i>Andrew J. Adamczyk, Agnes Derecskei-Kovacs, James R. Boulton, Michael P. Popule</i>	
(478b) A Computational Tool-Box for Pharmaceutical Chemical Development	175
<i>Yuriy Abramov</i>	
(478c) A Critical Evaluation of the Accuracy of Thermoset Models Created Using Atomistic Simulation Methods, Based on Gelation Studies	176
<i>David Rigby, Paul W. Saxe</i>	
(478d) Molecular Simulation of N-Octacosane – Water Gtl Mixtures in Nanopores at Elevated Temperature and Pressure	177
<i>Ioannis G. Economou, Konstantinos D. Papavasileiou, Zoi A. Makrodimitri, Jiaqi Chen, Gerard P. van der Laan, Ahmad Kalantar</i>	
(478e) Mind the Gap: Bridging Molecular and Fluid Dynamics Simulations in the Polyurethane Foam Industry	178
<i>Daniele Marchisio, Mohsen Karimi, Erik Laurini, Maurizio Fermeglia, Sabrina Pricl</i>	
(478f) How Uncertainty Quantification Renders Molecular Simulation a Quantitative Tool for Thermophysical Property Evaluation	179
<i>Richard A. Messerly, W. Vincent Wilding, Thomas A. Knotts</i>	
(478g) Alpha and Beta Glycine Nanocrystal Growth and Dissolution Kinetics in the Presence of an Electric Field through Molecular Dynamics - Towards Electric Field Controlled Crystallization	180
<i>Conor Parks, Andy Koswara, Nandkishor Nere, Shailendra Bordawekar, Hsien-Hsin Tung, Zoltan K. Nagy, Doraiswami Ramkrishna</i>	
(478h) Cheminformatic Selection of a Fluid for Use in a Single-Loop Thermal Control System	181
<i>Andrew L. Wagner, Ted J. Amundsen</i>	
(478j) Comparative Analysis of Biomimetic CO2 Hydration over Computationally Designed Ruthenium Cluster Decorated Graphene/Carbon Nanotube	182
<i>Manju Verma, Parag A. Deshpande</i>	
Impact Award: Inverse Design of Interactions for Assembly	183
<i>Thomas M. Truskett</i>	
Predicting Diffusion and Viscous Dissipation in Therapeutic Antibody Solutions	184
<i>James Swan</i>	
Characterizing Hydration at Nanostructured Surfaces – Applications to Materials Design and Protein Interaction Prediction	185
<i>Amish J. Patel</i>	
Young Investigator Award: Statistical Learning of Viral Fitness Landscapes for in silico Vaccine Design	186
<i>Andrew L. Ferguson</i>	
Computationally Connecting Organic Photovoltaic Performance to Atomistic Arrangements in Bulk Morphologies	187
<i>Eric Jankowski</i>	
(595a) Will Molecular Modeling Ever Become a Mainstream Chemical Engineering Tool?	188
<i>Edward J. Maginn</i>	
(595b) Expanding Molecular Simulation Use By Data/Code Sharing in Scientific Publishing	189
<i>John R. Kitchin</i>	
(595c) Integrated Upstream and Downstream Data Curation Tools As a Key to Enabling Reproducibility, Usability and Data Sharing	190
<i>Frederick R. Phelan, Thomas Rosch, Cheol Jeong, Brian Moroz, Sharief Youssef</i>	
(595d) High-Throughput Calculations of Molecular Properties in the MedeA® Environment	191
<i>Xavier Rozanska, Marianna Yannourakou, Philippe Ungerer, David Rigby, Clive M. Freeman, Paul W. Saxe</i>	
(595e) Application of Concepts from Modeling Integrated Computing for Molecular Simulation for Workflow Encapsulation	192
<i>Christoph Klein, Christopher R. Iacovella, János Sallai, Ákos Lédeczi, Clare McCabe, Peter T. Cummings</i>	
(595f) Making Molecular Modeling and Simulation a Mainstream Source of Data for Chemical Engineering Applications	193
<i>David A. Kofke, J. Ilja Siepmann, Joan F. Brennecke</i>	
(595g) The NIST Standard Reference Simulation Website: Reference Calculations and Evaluated Thermodynamics Properties to Aid Molecular Simulation Users	194
<i>Harold W. Hatch, William P. Krekelberg, Raymond D. Mountain, Vincent K. Shen, Daniel W. Siderius</i>	
(595h) What's the Molecular Simulation Checklist? Automating Both the Simulation and Research Choices to Achieve Better Robustness and Reproducibility	195
<i>Michael R. Shirts</i>	

(649a) Computational Study on the Thermal Degradation Mechanism and Gas Adsorption Properties of Mesoporous Silica MCM-41 after High Temperature Treatment	196
<i>Shenli Zhang, Roland Faller, Pieter Stroeve, Ricardo Castro</i>	
(649b) Methane-Hydrate Nucleation in Marine Environments: Insights from Molecular-Dynamics Strategies Exploring Free-Energy Landscapes	197
<i>Niall J. English, Marco Lauricella, Simone Meloni, Sauro Succi</i>	
(649c) Molecular Simulations of Wet Flue Gas Adsorption on 13X Zeolite	198
<i>Mark Purdue, Zhiwei Qiao, Jianwen Jiang, Shamsuzzaman Farooq</i>	
(649e) Exploring the Boundaries of Gas Adsorption Via Randomly Generated Porous Materials	199
<i>Christopher E. Wilmer, Alec R. Kaija</i>	
(649f) Interfacial Tension from Simulation and Theory	200
<i>Xiaoqun Mu, D. N. Asthagiri, Walter G. Chapman</i>	
(649g) Gas-Liquid Chromatography Column Selection By Molecular Simulation	201
<i>Qile Chen, J. Ilja Siepmann</i>	
(649h) Towards the Development of Single Atom Alloy Catalysts As a Means of Escaping Linear Scaling Relations	202
<i>Matthew Darby, E. Charles H. Sykes, Angelos Michaelides, Michail Stamatakis</i>	
(649i) Theory of Split Quantum Dot Formation in Strained-Layer Semiconductor Heteroepitaxy	203
<i>Lin Du, Dimitrios Maroudas</i>	
(649j) The Effect of Select Organic Compounds on Hydration of Portland Cement: Experimental and Molecular Dynamics Study	204
<i>Ojas Chaudhari, Joseph Biernacki, Scott Northrup</i>	
(681a) Accurate Property Prediction for Inorganic Materials with Machine Learning	205
<i>Olexandr Isayev</i>	
(681b) Comparing Molecules and Solids Across Structural and Alchemical Space	206
<i>Sandip De</i>	
(681c) Discriminative Neural Embeddings of Latent Variable Models for Molecular Property Prediction	207
<i>Hanjun Dai, Bo Dai, Le Song</i>	
(681d) On-the-Fly Heuristic Reordering Approach to Deterministic Optimization for Qualitative Chemical Property Prediction	208
<i>Jennifer M. Elward, Berend Christopher Rinderspacher</i>	
(681e) Machine Learning for Predicting Accurate Quantum Chemical Energies	209
<i>Pavlo O. Dral</i>	
(681f) Deductive and Inductive Modeling of Electronic Properties in the Organic Molecular Design Space	210
<i>Raghunathan Ramakrishnan</i>	
(681g) Sorting out a Process-Structure-Property Relationship in Polymer Organic Electronics	211
<i>Nils Persson, Michael McBride, Christopher A. Shartrand, Jye-Chyi Lu, Elsa Reichmanis, Martha A. Grover</i>	
(681h) Application of High Performance Computing and Machine Learning to Accelerate Material Discovery for Energy Capture and Storage	212
<i>Wesley Beckner, Jim Pfaendner</i>	
(681i) A Combinatorial Approach for Developing Minimally-Parameterized and Highly-Transferable Density Functionals	213
<i>Narbe Mardirossian, Martin Head-Gordon</i>	
(681j) Efficient K-Point Grid Generation through the Use of Informatics	214
<i>Pandu Wisesa, Tim Mueller</i>	
(681k) Machine Generated Coarse-Grained Force-Fields for Efficiently and Effectively Addressing Transferability	241
<i>Thomas Rosch, Paul Patrone, Frederick R. Phelan</i>	
(681l) Development of an Inter-Atomic Potential for Molecular Dynamics Simulations of Stanene Using a Genetic Algorithm Based Framework	242
<i>Mathew Cherukara, Badri Narayanan, Alper Kinaci, Kiran Sasikumar, Maria K. Y. Chan, Ross Harder, Subramanian K.R.S. Sankaranarayanan</i>	
(746a) A Lattice Kinetic Monte Carlo Method for Advective Systems	243
<i>Young Ki Lee, Talid Sinno</i>	
(746b) Continuous Fractional Component Monte Carlo in the Gibbs Ensemble	244
<i>Ali Poursaeidesfahani, Ariana Torres-Knoop, David Dubbeldam, Thijs Vlugt</i>	
(746c) Improved Coarse-Grained Models through Local Density Potentials Optimized with the Relative Entropy	245
<i>Tannoy Sanyal, M. Scott Shell</i>	
(746d) Explicit Nonlinear Collective Variables and Biased Molecular Dynamics Using Autoencoders	246
<i>Wei Chen, Andrew L. Ferguson</i>	
(746e) Solvent Activity in Electrolyte Solutions By Molecular Simulation of the Osmotic Pressure	247
<i>Maximilian Kohns, Steffen Reiser, Martin Horsch, Hans Hasse</i>	
(746f) Simulation Methods to Probe RNA Conformational Dynamics	248
<i>Rhiannon Jacobs, Harish Vashisth</i>	
(746g) Protracted Colored Noise Dynamics in Molecular Dynamics Simulations of Block Copolymers	249
<i>Benjamin Nation, Andrew J. Peters, Daniel Nicoloso, Peter Ludovice, Clifford L. Henderson</i>	
(746h) Efficient Simulation of the Hydrophobic Effect in Biological Self-Assembly	250
<i>Jens Glaser, Sharon C. Glotzer</i>	
(746i) First Principles Monte Carlo Simulations of Reaction Equilibria in Compressed Vapors	251
<i>J. Ilja Siepmann, Evgenii Fetisov</i>	

(746j) Replica-Exchange on-the-Fly Parameterization: Application of a High-Precision Free-Energy Method to Understanding the Roles of the M129V/D178N Polymorphisms in the Conformational Thermodynamics of Human Prion Protein	252
<i>Alexis Paz, Cameron F. Abrams</i>	
(757a) Molecular Dynamics Simulation of the Thermodynamics of Bismuth Telluride Exfoliation in Ionic Liquids	253
<i>Asghar Abedini, Thomas Ludwig, Zhongtao Zhang, C. Heath Turner</i>	
(757b) Tuning the Saw-Tooth Tensile Response and Toughness of Multiblock Copolymer Diamond Networks	255
<i>Christian Nowak, Fernando Escobedo</i>	
(757c) Impact of Surfaces Charge Distribution on the Mechanism of Heterogeneous Ice Nucleation	256
<i>Brittany Glatz, Sapna Sarupria</i>	
(757d) The Role of Dispersion Interactions, Electrostatics, and Entropy in the Interfacial Behavior of MoS₂	257
<i>Ananth Govind Rajan, Vishnu Sresht, Agilio A. H. Pádua, Michael S. Strano, Daniel Blankshtein</i>	
(757e) Interfacial Properties of Model Systems Using Molecular Dynamics Based Framework	258
<i>Kamlesh Jain, Andrew J. Schultz, Jeffrey R. Errington</i>	
(757f) Estimating Interfacial and Line Tensions Between Water, Vapor and Solid Substrates	259
<i>Suruchi Fialoke, Amish Patel</i>	
(757g) Molecular Dynamics Study on the Effects of Nanoscale Roughness on the Wear of Alkylsilane Monolayers	260
<i>Andrew Z. Summers, Christopher R. Iacovella, Peter T. Cummings, Clare McCabe</i>	
(757h) Reaxff Reactive Force Field Study of Cesium Adsorption in Micaceous Clay Minerals	261
<i>Muralikrishna Raju, Diana van Duin, Hiroki Nakamura, Masahiko Okumura, Masahiko Machida, Atsushi Fujiwara, Kento Mori, Adri van Duin</i>	
(757i) DFT Calculations of Multi-Coverage and Phase Adlayer Structure of Tryptophan on Cu(111)	262
<i>Rees B. Rankin</i>	
(757j) A Theoretical Study of Bulk and Inhomogeneous Hydration of Primary Amines	263
<i>Jia Fu, Shijie Sheng, Jianzhong Wu</i>	
(777a) Designing Functional Materials within the Materials Project	264
<i>Kristin Persson</i>	
(777b) Data Analytics and Machine Learning in Nanomaterials Discovery	265
<i>Michael Fernandez, Amanda S. Barnard</i>	
(777c) Describing the Diverse Geometries of Gold from Nanoclusters to Bulk a First-Principles Based Hybrid Bond Order Potential	266
<i>Badri Narayanan, Subramanian K.R.S. Sankaranarayanan</i>	
(777d) Topological Data Analysis of Nanoporous Materials Genome Using Pore-Geometry Recognition Technique	267
<i>Yongjin Lee, Berend Smit</i>	
(777e) Unraveling the Role of Pore Topology and Chemical Functionality on the Carbon Capture Performance of Metal-Organic Frameworks	268
<i>Diego Gomez-Gualdrón, Edwin Argueta, Randall Q. Snurr</i>	
(777f) An Automated Approach for Developing Graph-Theoretical Cluster Expansions of the Total Energy of Adsorbed Layers	269
<i>Emanuele Vignola, Stephan N. Steinmann, Michail Stamatakis, Phillippe Sautet</i>	
(777g) Property Prediction of Crystalline Solids from Composition and Crystal Structure	270
<i>Bruno A. Calfa, John R. Kitchin</i>	
(777h) Local Pattern Discovery for Uncovering Structure-Property Relationships of Materials	271
<i>Bryan R Goldsmith, Mario Boley, Luca M. Ghiringhelli, Matthias Scheffler</i>	
(777i) Alloy Catalyst Discovery Using Computational Alchemy	272
<i>Karthikeyan Saravanan, O. Anatole von Lilienfeld, John A. Keith</i>	
(777j) To Address Surface Reaction Network Complexity Using Machine Learning, Scaling Relations, and DFT Calculations	273
<i>Zachary Ulissi, Jens K. Nørskov, Thomas Bligaard, Andrew Medford</i>	
(777k) Machine-Learning Acceleration of the Exploration of Potential Energy Surface within Amp	274
<i>Alireza Khorshidi, Andrew A. Peterson</i>	
Author Index	