

# **Computational Molecular Science and Engineering Forum 2017**

Core Programming Area at the 2017 AIChE Annual Meeting

Minneapolis, Minnesota, USA  
29 October – 3 November 2017

ISBN: 978-1-5108-5807-7

**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© (2017) by AIChE  
All rights reserved.

Printed by Curran Associates, Inc. (2018)

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](http://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](mailto:curran@proceedings.com)  
Web: [www.proceedings.com](http://www.proceedings.com)

## TABLE OF CONTENTS

<b>(1a) On-Boarding Computational Scientists with Bash, Git, and Python .....</b>	1
<i>Eric Jankowski</i>	
<b>(1b) Mosdef: Molecular Simulation and Design Framework.....</b>	2
<i>Christoph Klein, J. Sallai, Andrew Z. Summers, Christopher R. Iacovella, A. Ledeczi, Clare McCabe, Peter T. Cummings</i>	
<b>(1c) Managing Data Spaces, Performing MD, and Analyzing Trajectories with Signac, HOOMD-Blue, and Freud .....</b>	3
<i>Carl Simon Adorf, Joshua A. Anderson, Eric S. Harper, Sharon C. Glotzer</i>	
<b>(1d) How to Recognize Garbage .....</b>	4
<i>Michael Shirts</i>	
<b>(1e) How to Use the Atomistic Monte Carlo Package Cassandra: Liquid Phase Properties and Vapor-Liquid Phase Equilibria .....</b>	5
<i>Edward J. Maginn, Eliseo Marin-Rimoldi, Jindal K. Shah, Ryan Gotchy Mullen</i>	
<b>(1f) Using Python to Standardize and Format Input to Popular Molecular Simulation Software .....</b>	6
<i>Coray M. Colina, Michael E. Fortunato</i>	
<b>(1g) Quantifying Uncertainty in Molecular Simulations .....</b>	7
<i>David A. Kofke, Andrew J. Schultz</i>	
<b>(39a) Contact Freezing Vs. Surface Freezing in Water .....</b>	8
<i>Amir Haji-Akbari</i>	
<b>(39b) Modeling the Homogeneous and Heterogeneous Nucleation of Crystals of Ionic Liquids in Different Environments.....</b>	9
<i>Yan Shen, Xiaoxia He, Erik E. Santiso, Francisco R. Hung</i>	
<b>(39c) Using Transition Path Sampling to Determine the Mechanism of the Fcc-Hcp Phase Transformation in Solid Ar .....</b>	10
<i>Bingxi Li, Artem Oganov, Roland Faller</i>	
<b>(39d) Using Metadynamics to Resolve and Characterize Complex Reactions at the Molecular Scale .....</b>	11
<i>Christopher Fu, Jim Pfaendtner</i>	
<b>(39e) Improving Ab Initio Molecular Dynamics Simulations of Water with Experimental Data .....</b>	12
<i>Andrew White</i>	
<b>(39f) Predicting Hydrogen-Deuterium Exchange Rates in Proteins Using Molecular Dynamics Simulations.....</b>	13
<i>Harish Vashisth</i>	
<b>(39g) Using Semidefinite Programming to Calculate Bounds on Stochastic Chemical Kinetic Systems.....</b>	14
<i>Garrett R. Dowdy, Paul I. Barton</i>	
<b>(39h) Automated Discovery of Reaction Pathways for the Combustion of Alternative Fuel Candidates .....</b>	26
<i>Ahmed E. Ismail</i>	
<b>(70a) A Generic Coarse-Grained Model of Influenza Budding: What Can We Learn? .....</b>	27
<i>Jesper J. Madsen, John M. A. Grime, Gregory A. Voth</i>	
<b>(70b) Allosteric Effects of Gold Nanoparticles on Human Serum Albumin .....</b>	28
<i>Qing Shao, Carol K. Hall</i>	
<b>(70c) Self-Assembly of Proteins: The Role of Shape and Specific Interaction.....</b>	29
<i>Jens Glaser, Sharon C. Glotzer</i>	
<b>(70d) Predictive Design of Next-Generation Nanomaterials and Devices Via Bottom-up Approaches .....</b>	30
<i>Trung Nguyen</i>	
<b>(70e) Solvation of Self-Assembled Complexes: Using Molecular Simulations to Probe Energetics, Structure, and Dynamics.....</b>	31
<i>Kevin R. Hinkle, Frederick R. Phelan Jr.</i>	
<b>(70f) Level Set Strategy for Self Consistent Field Theory .....</b>	32
<i>Gaddiel Ouaknin</i>	
<b>(70g) Simulations of Nonlinear Flows in Nonequilibrium Complex Liquids .....</b>	33
<i>Rui Zhang</i>	
<b>(70h) Employing a Multipole Approximation in a Hybrid Fluid Via Relative Resolution .....</b>	34
<i>Aviel Chaimovich, Christine Peter, Kurt Kremer</i>	
<b>(70j) Quantitatively Reliable Molecular Modeling and Simulation of Vapor-Liquid Equilibria.....</b>	35
<i>Martin T. Horsch</i>	
<b>(84a) Atomistic Simulations of Ordered and Disordered Carbons: "Mimicking" Versus "Targeting" .....</b>	36
<i>Roland J.-M. Pellennq</i>	

<b>(84b) Graphene Oxide Membranes: A Molecular Simulation Approach .....</b>	37
<i>Christopher Williams, Paola Carbone, Flor R. Siperstein</i>	
<b>(84c) Polyethylene Oxide (PEO) in a Polyethylene (PE) Framework: A Simple Model for Simulation Studies of Scaling and Solvent Effects on Polymers in an Open Framework.....</b>	38
<i>Kwong-Yu Chan, Liangxu Xie, Nicholas Quirke</i>	
<b>(84d) Molecular Understanding and Design of Zwitterionic Materials .....</b>	39
<i>Shaoyi Jiang</i>	
<b>(84e) Interfacial Transport of Protons on a 2-Dimensional Functionalized Graphane Surface.....</b>	40
<i>J. Karl Johnson, Abhishek Bagussetty, Bridget Derksen, Pabitra Choudhury</i>	
<b>(84f) Gas Adsorption Behavior in Ionic Polyimide Composite Membranes .....</b>	41
<i>C. Heath Turner, Asghar Abedini, Ellis Crabtree, Jason E. Bara</i>	
<b>(84g) Computational Simulation of Supported Nanocatalysts Under Realistic Conditions .....</b>	42
<i>Jian-Guo Wang</i>	
<b>(147a) Metastable Phase Transitions.....</b>	43
<i>Pablo G. Debenedetti</i>	
<b>(147b) Computational Investigation of Multipolar Colloidal Particle.....</b>	44
<i>David M. Rutkowski, Ryan C. Maloney, Orlin D. Velez, Sabine H. L. Klapp, Carol K. Hall</i>	
<b>(147c) Interfacial Tensions from SAFT: Connecting Equations of State to Molecular Simulations .....</b>	45
<i>Erich A. Muller</i>	
<b>(147d) Generalized Gibbs Free Energy of Confined Nanoparticles .....</b>	46
<i>Xiaohua Lu</i>	
<b>(147e) Molecular Modeling of Polymeric Systems .....</b>	47
<i>Coray M. Colina</i>	
<b>(147f) Effect and Regulation of Surface Wettability on Molecular Transport and Reaction.....</b>	48
<i>Shuangliang Zhao, Honglai Liu</i>	
<b>(152a) Digital Alchemy for Assembly Engineering .....</b>	49
<i>Sharon C. Glotzer</i>	
<b>(152b) Improved Algebraic, Numerical, and Graphical Representations in Fluid Mechanics .....</b>	50
<i>Stuart W. Churchill, James C. Hill</i>	
<b>(152c) The Scaling of Turbulence Near the Wall and the Churchill Turbulent Flux Correlation: Insights with Lagrangian Simulations .....</b>	51
<i>Dimitrios V. Papavassiliou, Quoc T. Nguyen, Chiranth Srinivasan</i>	
<b>(152d) Flow Boiling Using a Piranha Pin Fin Heat Sink .....</b>	52
<i>Cory Woodcock, Xiangfei Yu, Yoav Peles, Joel L. Plawsky</i>	
<b>(152e) Transport Problems in the Spirit of Stuart Churchill for Teaching and Research at the University of Michigan .....</b>	53
<i>Ronald G. Larson, Claudio Vilas Boas Favero</i>	
<b>(176a) Solve this! Fundamental Approach to Problem Solving in Industrial Processes I (Invited Talks) .....</b>	54
<i>Zdravko Stefanov, Paul Chauvel, Jr., Eldad Herceg, Dana A. Livingston</i>	
<b>(192a) Comparison of PRISM Theory and Molecular Dynamics Simulations for Studying Assembly in Block Copolymer Solutions of Varying Sequences and Composition.....</b>	55
<i>Ivan Lyubimov, Daniel J. Beltran-Villegas, Arthi Jayaraman</i>	
<b>(192aa) Novel Computational/Experimental Apporaches to DNA/Proteins Interactions.....</b>	56
<i>Sabrina Priol, Erik Laurini, Maurizio Fermeglia, Domenico Marson, Enzo Di Fabrizio, Monica Marini</i>	
<b>(192ab) Wiggling, Crowding, Self-Assembling, Synthesis and Activity of Computer-Designed Nanovectors for Gene and Drug Delivery.....</b>	57
<i>Erik Laurini, Maurizio Fermeglia, Silvia Brich, Domenico Marson</i>	
<b>(192ac) New Anti-Mycobacterium Agents in Combination with Pgp Inhibitors: A Multidisciplinary Approach to Face an Old Re-Emerging Disease with New Tools .....</b>	58
<i>Erik Laurini, Suzana Aulic, Maurizio Fermeglia, Domenico Marson, Irene Briguglio, Roberta Ibba, Antonio Carta, Sabrina Priol</i>	
<b>(192ad) Qsars for Predicting Adipose:Blood Partitioning of Industrial Chemicals.....</b>	59
<i>Krystalia Papadaki, Spyros Karakitsios, Dimosthenis Sarigiannis</i>	
<b>(192ae) Pharmacometabonomics Approach for Early Prediction of Neuropathy.....</b>	60
<i>Parul Verma, Jamie Renbarger, Jodi Skiles, Bruce Cooper, Doraiswami Ramkrishna</i>	
<b>(192af) A Theoretical Study of the Activation of Hydrogen and Methane By Frustrated Lewis Pairs .....</b>	61
<i>Marcos Becerra, Misael Real-Enriquez, Luis Rincon</i>	
<b>(192ag) Differences in Relative Free Energy Versus Temperature Curves for Small Organic Molecules between Quantum Mechanical and Classical Potentials.....</b>	62
<i>Natalie Schieber, Nathan Abraham, Eric Dybeck, Michael Shirts</i>	

<b>(192ah) Density Functional Theory Screening of Metal Catecholates for Adsorption of Toxic Pnictogen Hydride Gases .....</b>	63
<i>N. Scott Bobbitt, Randall Q. Snurr</i>	
<b>(192ai) Mechanism of Sodium Adsorption on N-Doped Graphene Nanoribbons .....</b>	64
<i>Hong Woo Lee, Hye Sook Moon, Je Moon Yun, Kwang Ho Kim, Seung Geol Lee</i>	
<b>(192aj) Influence of Solvent on the Thermodynamics of Molecular Adsorption on Metal Surfaces .....</b>	65
<i>Tonnam Balankura, Kristen Fichthorn</i>	
<b>(192al) Computational Discovery of New Materials and Processes for Industrial Separations .....</b>	66
<i>Mansi S. Shah, Michael Tsapatsis, J. Ilja Siepmann</i>	
<b>(192an) Molecular Simulations of Fullerene Stabilization in Water By Fullerene-Oxides.....</b>	67
<i>Kendra Noneman, Eric Jankowski</i>	
<b>(192ao) Interplay between Crystallization and Glass Transition in Bimetallic Nanoalloys .....</b>	68
<i>Solene Bechelli, Caroline Desgranges, Jerome Delhommelle</i>	
<b>(192ap) Molecular Simulations of Bubble Formation in Metastable Liquids.....</b>	69
<i>Brittany Gonzalez, Caroline Desgranges, Jerome Delhommelle</i>	
<b>(192aq) Molecular Simulation of Gas Adsorption in Metal-Organic Frameworks .....</b>	70
<i>Gopalsamy Karuppasamy, Caroline Desgranges, Jerome Delhommelle</i>	
<b>(192ar) Leveraging Heterostructural Alloying to Design Metastable Nitrides with Improved Piezoelectric Properties .....</b>	71
<i>Samantha L. Millican, Kevin Talley, Alan W. Weimer, Andriy Zakutayev, Charles B. Musgrave, Geoff Brennecke, Aaron Holder</i>	
<b>(192as) Discovery of High-Performing MOFs Via High-Throughput Computation and Machine Learning .....</b>	72
<i>Alauddin Ahmed</i>	
<b>(192at) First-Principles Studies of the Interactions Between Chemical Species inside Vanadium Redox Flow Batteries .....</b>	73
<i>Nadia N. Intan, Konstantin Klyukin, Vitaly Alexandrov</i>	
<b>(192au) Dehydrogenation Mechanism of Liquid Organic Hydrogen Carrier Materials: A Density Functional Theory Study.....</b>	74
<i>Jae Yul Lim, Hyunguk Kwon, H. Shaun Kwak, Jeong Woo Han</i>	
<b>(192av) The Crystal Structure and Surface Composition of Coalescing Ag-Au Nano-Alloys By Molecular Dynamics Simulations.....</b>	75
<i>Eirini Goudeli, Sotiris E. Pratsinis</i>	
<b>(192ax) First-Principles Study of Atomistic Mechanisms in All-Vanadium Redox Flow Batteries .....</b>	76
<i>Zhen Jiang, Konstantin Klyukin, Vitaly Alexandrov</i>	
<b>(192ay) Solvation Dynamics and Energetics of Single-Walled Carbon Nanotubes (SWCNTs) in Water/Alcohol Mixtures.....</b>	77
<i>Kevin R. Hinkle, Frederick R. Phelan Jr.</i>	
<b>(192az) Effect of Liquid-Liquid and Solid-Liquid Interfacial Resistance on Heat Transfer in Nanomaterials .....</b>	78
<i>Sohail Murad, Ishwar K. Puri</i>	
<b>(192b) Molecular Dynamics of Inorganic and Polymer Interface with Force-Field Parameter Based on DFT Simulation.....</b>	79
<i>Hiroya Nitta, Kosuke Ohata, Kenta Chaki, Taku Ozawa</i>	
<b>(192bb) Multi Metric 3D Protein Descriptors: The Correlation Impact of Algebraic Forms and Its Analysis.....</b>	80
<i>Julio Teran, Yovani Marrero-Ponce</i>	
<b>(192bc) Accurate Methods to Describe System-Specific Polarization and Dispersion Energies .....</b>	81
<i>Thomas A. Manz, Nidia Gabaldon Limas, Taoyi Chen, Daniel J. Cole</i>	
<b>(192bd) Applications of Atomistic Machine Learning for Estimating Adsorbate Free Energy and Entropy on Late-Transition Metal Surfaces.....</b>	82
<i>Prateek Mehta, Andrew Lehmer, Anshumaan Bajpai, Kurt Frey, William F. Schneider</i>	
<b>(192be) Reconstructing Ancient Sequences to Understand the Structure and Function Relationships of Modern Proteins.....</b>	83
<i>Zahra Shamsi, Alexander Moffett, Diwakar Shukla</i>	
<b>(192bf) Improved Thermal Gradient Quasiharmonic Approximations for Thermodynamic Properties of Organic Crystals with the Inclusion of Anisotropy .....</b>	84
<i>Nathan Abraham, Eric Dybeck, Natalie Schieber, Michael Shirts</i>	
<b>(192bg) Mosdef, a Python-Based Molecular Simulation and Design Framework.....</b>	85
<i>Justin Gilmer, Christoph Klein, János Sallai, Andrew Z. Summers, Christopher R. Iacovella, Ákos Lászlódeczi, Clare McCabe, Peter T. Cummings</i>	

<b>(192bh) Screening Self-Assembled Monolayers for Lubrication Properties: Trends and Pitfalls .....</b>	86
<i>Christopher R. Iacovella, Christoph Klein, Trevor J. Jones, Clare McCabe, Peter T. Cummings</i>	
<b>(192bi) Addressing Discrepancies in Hydrogen Abstraction By Ooh Radical Via Automatic Transition State Theory Calculations .....</b>	87
<i>Nathan Harms, Richard H. West</i>	
<b>(192bj) Development of the Parallel Monte Carlo Simulation Engine Gomc .....</b>	88
<i>Mohammad Barhaghi, Jason R. Mick, Younes Nejahi, Yuanzhe Li, Loren Schwiebert, Jeffrey J. Potoff</i>	
<b>(192bl) Theoretical Study Energetic Ionic Salts Composed of Nitrogen Bridge 3,3'-dinitro-5,5'-bis-1,2,4-triazole-1,1'-diolate Anion and Various Cations .....</b>	89
<i>Guolin Xiong, Weihua Zhu, Heming Xiao</i>	
<b>(192bm) Structural Transformations and Absorption Properties of Crystalline4,10-dinitro-2,6,8,12-tetraoxa-4,10-diazaisowurtzitane under High Pressures.....</b>	102
<i>Dong Xiang, Weihua Zhu</i>	
<b>(192c) Comprehensive Generation of Libraries of Lignin Structures As an Exploration of Lignin Space .....</b>	129
<i>Lauren Dallon, Abraham Yanez-McKay, Wenjun Li, Ross Mabon, Linda J. Broadbelt</i>	
<b>(192d) Understanding the Nanoscopic Structure of Lyotropic Liquid Crystal Membranes Using Molecular Dynamics Simulations .....</b>	130
<i>Benjamin J. Coscia, Michael Shirts</i>	
<b>(192e) Thermodynamics of Block Polymers - Monte Carlo Simulations and Self-Consistent Field Theory Study.....</b>	131
<i>Akash Arora, Frank S. Bates, Kevin D. Dorfman</i>	
<b>(192f) Refinement of Techniques in Molecular Modeling of Multicompartment Nanoreactors .....</b>	132
<i>Kayla Hendrickson, Nicholas Bond, Seungmin Lee, Connor Callaway, Parveen Sood, Seung Soon Jang</i>	
<b>(192g) Rapid and Accurate Property Prediction for Polymer Systems Using Atomistic-Scale Simulation .....</b>	133
<i>Andrea R. Browning, Thomas J. L. Mustard, Jeffrey Sanders, Mathew D. Halls, Alexander Goldberg, H. Shaun Kwak, Stephen Christensen, Jacob Gavartin, Morisato Tsuguo</i>	
<b>(192h) Flow Properties of Model Alkanes in Nanopores .....</b>	134
<i>Irais Valencia-Jaime, Caroline Desgranges, Jerome Delhommelle</i>	
<b>(192i) Pure and Mixed Gas Absorption in Nonideal Binary Ionic Liquid Mixtures, a Molecular Simulation Study.....</b>	135
<i>Utkarsh Kapoor, Jindal K. Shah</i>	
<b>(192j) Construction of a Hydrogel System for Bioadsorption and Bioseparations By Molecular Modeling and Simulation .....</b>	136
<i>Matthew Senter, Jee-Ching Wang</i>	
<b>(192k) Modeling Alkane Partitioning and Phase Behavior in Non-Permeable and Permeable Slit Pores .....</b>	137
<i>Jinlu Liu, Walter G. Chapman</i>	
<b>(192o) Enhancing the Oxidation of Toluene with External Electric Fields: A Reactive Molecular Dynamics Study .....</b>	138
<i>Shen Tan, Tao Xia, Yao Shi, Yi He</i>	
<b>(192p) Molecular Simulation of Ionic Polyimides and Ionic Liquid Composites for Gas Separation .....</b>	139
<i>Asghar Abedini, C. Heath Turner, Jason E. Bara, Ellis Crabtree</i>	
<b>(192q) Molecular Simulation of Ionic Liquid Mixtures: Applications to Capacitive Energy Storage.....</b>	140
<i>Matt Thompson, Katherine L. Van Aken, Robert Sacci, Justin Neal, Jianzhong Wu, Yury Gogotsi, Peter T. Cummings</i>	
<b>(192r) Molecular Simulation of Ionic Liquid Systems: Effects of Solvation and Humidification .....</b>	141
<i>Matt Thompson, Felix Tiet, Naresh C. Otsi, Boris Dyatkin, Katherine L. Van Aken, De-En Jiang, Yury Gogotsi, Eugene Mamontov, Peter T. Cummings</i>	
<b>(192s) Aerosol Formation in Post Combustion CO<sub>2</sub> Capture Columns - Molecular Dynamic Simulation .....</b>	142
<i>Dhawal Shah, Nardana Bazybek, Tomiris Boltaikhanova</i>	
<b>(192t) Molecular Simulation of Transport of DNA Grafted Nanoparticles .....</b>	143
<i>James McLaughlin, Simona Ciobotarescu, Caroline Desgranges, Jerome Delhommelle</i>	
<b>(192u) Protein Adsorption on Surfaces: The Role of Forcefield and Surface Ions.....</b>	144
<i>Arushi Prakash, Kayla Sprenger, Jim Pfaendtner</i>	
<b>(192v) Scaling of Peptide Sequence-Dependent Hydrophobic Interactions from Experiment and Simulation .....</b>	145
<i>Jacob I. Monroe, Philipp Stock, Thomas Utzig, David J. Smith, Markus Valtiner, M. Scott Shell</i>	
<b>(192w) Mapping of Gas Diffusion Pathways in [FeFe]-Hydrogenase.....</b>	146
<i>Mohammadjavad Mohammadi, Harish Vashisth</i>	

<b>(192x) Studying the Structure and Dynamics of Amyloid<math>\beta</math>(21-30) with Experiments and Simulations.....</b>	147
<i>Dilnoza Amirkulova, Maghesree Chakraborty, Andrew White</i>	
<b>(192y) Solute Transport across Blood-Brain Barrier Tight Junction Pores .....</b>	148
<i>Flaviyan Jerome Irudayanathan, Shikha Nangia</i>	
<b>(192z) Capturing Differences in Dynamics of Structurally Similar Signaling Proteins.....</b>	149
<i>Hossein Mohammadiarani, Harish Vashisth</i>	
<b>(218a) Rational Design of Alloyed Materials for Energy Conversion.....</b>	150
<i>Liang Zhang</i>	
<b>(218b) Climbing the Volcano: Active-Site Engineering at the Atomic Scale .....</b>	154
<i>Joseph H. Montoya</i>	
<b>(218c) Developing Ab Initio Methodology for Advancing Catalytic Reactions .....</b>	155
<i>Eric Walker</i>	
<b>(218d) First-Principles-Derived Structure-Energy Relationship for Surface Oxides .....</b>	156
<i>Alexander V. Mironenko, Dionisios G. Vlachos</i>	
<b>(218e) First-Principles Based Design of Reaction Conditions for the Catalytic Conversion of Methane to Methanol over Cu-Exchanged SSZ-13.....</b>	157
<i>Florian Goltl, Manos Mavrikakis</i>	
<b>(218f) Reaction Ensemble Monte Carlo Simulations of Xylene Isomerization Under Confinement .....</b>	158
<i>Ryan Gotchy Mullen, Edward J. Maginn</i>	
<b>(218g) Understanding Separation and Catalysis in Nanoporous Materials.....</b>	159
<i>Peng Bai</i>	
<b>(218h) Modeling Self-Assembly of Metal-Organic Frameworks with Enhanced Sampling Techniques.....</b>	160
<i>Yamil J. Colon, Ashley Guo, Lucas Antony, Kyle Hoffmann, Juan J. De Pablo</i>	
<b>(218i) Computationally-Efficient High-Throughput Screening of Metal-Organic Frameworks for Hydrogen Storage .....</b>	161
<i>N. Scott Bobbitt, Arun Gopalan, Benjamin Bucior, Jiayi Chen, Randall Q. Snurr</i>	
<b>(218j) Effects of Ion Self-Energy on the Double Layer Structure and Properties at the Dielectric Interface .....</b>	162
<i>Rui Wang</i>	
<b>(260a) Molecular Investigation into the Transport across the Blood-Brain Barrier Interface [Invited Talk].....</b>	163
<i>Shikha Nangia, Flaviyan Jerome Irudayanathan, Nan Wang, Xiaoyi Wang</i>	
<b>(260b) Adsorption and Self-Assembly of Surfactants on Metallic Surfaces Studied Using Molecular Simulations.....</b>	164
<i>Sumit Sharma, Xueying Ko</i>	
<b>(260c) Modeling Alkane Partitioning and Phase Behavior on Graphite Pores: A Discussion on Dispersion Free Energy Formalism.....</b>	165
<i>Jinlu Liu, Walter G. Chapman</i>	
<b>(260d) Effect of Solvent on the Binding Energies of Molecules on Metal Surfaces .....</b>	166
<i>Tonnam Balankura, Kristen Fichthorn</i>	
<b>(260e) Tuning Proximal Water Diffusion Via Silanol Patterning on Quartz Surfaces .....</b>	167
<i>Jacob I. Monroe, Alex Schrader, Song-I Han, M. Scott Shell</i>	
<b>(260f) Molecular Dynamics Studies of the Effects of Ionic Liquid Molecular Properties and Particle Concentration on the Behavior of Nanoparticles at the Ionic Liquid/Water Interface .....</b>	168
<i>Stella D. Nickerson, Lenore L. Dai</i>	
<b>(260h) Evaporation Induced Nucleation of NaCl in Clay Minerals: Mechanism and Potential Sites.....</b>	169
<i>Hassan Dashtian, Haimeng Wang, Muhammad Sahimi</i>	
<b>(260i) Computational Investigation of the Role of Topology and Functionalization on ZIF Stability.....</b>	170
<i>Rebecca Han, Souryadeep Bhattacharyya, David Sholl, Sankar Nair</i>	
<b>(304a) Multiconfiguration Pair-Density Functional Theory for Computational Catalysis.....</b>	179
<i>Laura Gagliardi, Donald G. Truhlar</i>	
<b>(304b) Quantum Mechanical Description of Excited-State Heterogeneous Catalysis Via Embedded Correlated Wavefunction Methods .....</b>	180
<i>John Mark P. Martirez, Emily A. Carter</i>	
<b>(304c) Incorporation of Linear Scaling Relations into Automatic Mechanism Generation for Heterogeneous Catalysis.....</b>	181
<i>Richard H. West, C. Franklin Goldsmith</i>	
<b>(304d) DFT+U-Inspired Functional for Improved Modeling of Molecules and Solids .....</b>	182
<i>Alexander V. Mironenko, Dionisios G. Vlachos</i>	
<b>(304e) Development of "Surrogate" Hybrid Functionals Based on Electron Density Convolutions .....</b>	183
<i>Andrew Medford, Ray Lei</i>	

<b>(304f) Accurate Correction of DFT Delocalization Error in Transition Metal Catalysis .....</b>	184
<i>Qing Zhao, Terry Z. H. Gani, Akash Bajaj, Heather J. Kulik</i>	
<b>(304g) The Effects of Oxidation and Transition Metal-Doping on the Structure and Properties of Pt-Ni Nanoparticles .....</b>	185
<i>Liang Cao, Tim Mueller</i>	
<b>(304h) The Influence of Hubbard U Parameter in Simulating Adsorption and Reactivity on CuO Surface(s): A Combined Theoretical and Experimental Study.....</b>	186
<i>Kartavya Bhola, Jithin John Varghese, Liu Dapeng, Yan Liu, Samir H. Mushrif</i>	
<b>(377a) Simulating Solvent Effects in Catalytic Systems.....</b>	187
<i>Matthew Neurock, Peng Bai, Chottithai Sanpitaksere</i>	
<b>(377b) Electronic Excitations in Thermal Heterogeneous Catalysis.....</b>	188
<i>Matthew M. Montemore, Robert Hoyt, Grigory Kolesov, Eftimios Kaxiras</i>	
<b>(377c) Large-Scale Nonadiabatic Molecular Dynamics Enabled By Machine Learning.....</b>	189
<i>Jiamin Wang, Hongliang Xin</i>	
<b>(377d) Modeling of Segregation on Au-Pd (111) Surfaces with Monte Carlo Simulations and Neural Network Atomic Potentials .....</b>	190
<i>Jacob R. Boes, John R. Kitchin</i>	
<b>(377e) Accelerating Electronic Structure Calculations with Machine Learning.....</b>	191
<i>Andrew A. Peterson, Alireza Khoshidi</i>	
<b>(377f) A Data-Driven in silico Research Paradigm for the Rational Design of Catalyst Systems and the Exploration of Chemical Space.....</b>	192
<i>Johannes Hachmann</i>	
<b>(377g) Overcoming the Compromise between Accuracy and Efficiency in Modelling Catalytic Kinetics .....</b>	193
<i>Miguel Pineda, Michail Stamatakis</i>	
<b>(377h) CO Adsorption on Platinum and Cobalt: Site Preference and Coverage Effects.....</b>	200
<i>G. T. Kasun Kalhara Gunasooriya, Mark Saeys</i>	
<b>The Pressure-Velocity Relation .....</b>	201
<i>Scott Bair</i>	
<b>Viscosity Predictions using Nonequilibrium Molecular Dynamics Simulations.....</b>	219
<i>Jerome Delhommele, Caroline Desgranges</i>	
<b>Elastohydrodynamic Lubrication and Glassy Flow: Linking Experiments and Simulations at High Rates and Pressures.....</b>	220
<i>Vikram Jadho, Mark Robbins</i>	
<b>(415a) The Surprising Accuracy of Dispersion-Corrected Ggas in the Prediction of Dissociation Barriers on Transition Metal Surfaces .....</b>	221
<i>Shaama Mallikarjun Sharada, Thomas Bligaard, Alan C. Luntz, Geert-Jan Kroes, Jens Norskov</i>	
<b>(415b) Adsorbate Vibrations on Transition Metal Surfaces: Applications and Theory .....</b>	222
<i>Joshua Lansford, Dionisios G. Vlachos</i>	
<b>(415c) Genetic Algorithm Enhanced By Atomistic Neural Network: Pt Clusters at the H2 Atmosphere as an Example .....</b>	231
<i>Geng Sun, Phillippe Sautet</i>	
<b>(415d) Prediction of Chemisorption Energies By Gaussian Processes .....</b>	232
<i>Martin H. Hansen, Paul C. Jennings, Thomas Bligaard</i>	
<b>(415e) New Computational Tools for High-Throughput Discovery in Transition Metal Catalysis .....</b>	233
<i>Terry Z. H. Gani, Jon Paul Janet, Heather J. Kulik</i>	
<b>(415f) More Accurate Depiction of Adsorption Energy on Transition Metals Using Work Function As One Additional Descriptor .....</b>	234
<i>Xiaochen Shen, Yanbo Pan, Bin Liu, Jinlong Yang, Jie Zeng, Zhenmeng Peng</i>	
<b>(415g) Molecular Simulation Study of How the Structure of Liquid Water Affects the Free Energies of Adsorption and Reaction in Aqueous Phase Heterogeneous Catalysis .....</b>	235
<i>Xiaohong Zhang, Rachel Getman</i>	
<b>(428a) Top Ten Mistakes Applying Computational Chemistry in Industry .....</b>	236
<i>Brian K. Peterson</i>	
<b>(428b) Atomic-Level Insights into Chemical Additives Used for Silicon-Containing Film Removal during Integrated Circuit Manufacturing.....</b>	237
<i>Andrew J. Adamezyk, Wen Dar Liu, Yi Chia Lee</i>	
<b>(428c) Thiohypoidous Acid (HSI) Formation and Its Role As an Intermediate in H2 Production .....</b>	238
<i>Phalgun Lolur, Ryan J. Gillis, William H. Green</i>	
<b>(428d) Computational Design of Thermodynamically Stable Metal Nanoparticles .....</b>	239
<i>Giannis Mpourmpakis</i>	

<b>(428e) Understanding the Geometrical and Electronic Properties of Imidazolium-Based Ionic Liquids in the Presence of Amino Acid Substituted Metal Porphyrins.....</b>	240
<i>Atiya Banerjee, Jindal K. Shah</i>	
<b>(428f) Towards the Prediction of the Liquid Phase Oxidation of Aromatics - an Experimental and Modeling Study for Toluene Autoxidation .....</b>	241
<i>M. Matrat, Detlev C. Mielczarek, Arij Ben Amara, Perrine Wund, Yvan Bouyou, Laurie Starck</i>	
<b>(428g) Multiscale Molecular Dynamics Simulations of Asphaltenes in Crude Oils Based on the SAFT-<math>\gamma</math> Mie Force Field .....</b>	244
<i>Jason Law, M. Guadalupe Jimenez-Serratos, Erich A. Muller</i>	
<b>(428h) Evaluating the Consistency and Accuracy of COSMO-RS Based Free Energy Predictions .....</b>	245
<i>Jens Reinisch, Andreas Klamt</i>	
<b>(469a) Support Effects in Heterogeneous Catalysis Using Au Nanoparticles on Oxides: A DFT Analysis.....</b>	246
<i>Paulami Majumdar, Yanran Cui, Fabio H. Ribeiro, Jeffrey Greeley</i>	
<b>(469b) Coordination-Based Descriptors for Rational Design of Metal Nanocatalysts .....</b>	247
<i>Siwen Wang, Hongliang Xin</i>	
<b>(469c) Theoretical Investigation of the Ring Opening Mechanism of Cyclohexanes on Ir Surfaces.....</b>	248
<i>Kushal Ghale, Ye Xu</i>	
<b>(469d) CO<sub>2</sub> Reduction on the Nickel Surface.....</b>	249
<i>Wei Lin, George C. Schatz</i>	
<b>(469e) Designing Cu-Based Bimetallic Nanoparticles for CO<sub>2</sub> Activation .....</b>	250
<i>James Dean, Giannis Mpourmpakis</i>	
<b>(582h) Understanding Heterogeneous Catalyst Deactivation By Biogenic Impurities on Ni (111) Surface and Bimetallic Alloy .....</b>	251
<i>Madhulika Gupta, Tuhin Suvra Khan, Shelaka Gupta, Md. Imteyaz Alam, Manish Agarwal, M. Ali Haider</i>	
<b>(469g) Determination of Iridium Alloy Properties for Catalytic Applications .....</b>	252
<i>Lida Mehdizadegan Namin, N. Aaron Deskins</i>	
<b>(508a) Elucidating Molecular Details of Protein Liquid-Liquid Phase Separation By a Coarse-Grained Model.....</b>	253
<i>Gregory L. Dignon, Wenwei Zheng, Robert Best, Jeetain Mittal</i>	
<b>(508b) Real-Time Electron Dynamics of Large Complex Systems from a Density Functional Tight Binding Approach.....</b>	254
<i>Bryan M. Wong</i>	
<b>(508c) Computational Investigation of Ionic Liquids Nanostructure Formation at a Mesoscale.....</b>	255
<i>Sergiy Markutsya, Justin B. Haskins, John W. Lawson</i>	
<b>(508d) Ultra-Coarse-Grained Modeling of ATP Hydrolysis in an Actin Filament.....</b>	256
<i>Harshwardhan H. Katkar, Aram Davtyan, Aleksander E. P. Durumeric, Glen M. Hocky, Gregory A. Voth</i>	
<b>(508e) Validation of Biomolecular Force Fields Regarding Structural and Thermodynamic Properties of Cyclodextrins and Their Complexes.....</b>	257
<i>Julia Gebhardt, Daniel Markthaler, Niels Hansen</i>	
<b>(508f) Optimal Probes: A Machine Learning Platform for Å Design of Experimental Probes for Protein Dynamics.....</b>	258
<i>Diwakar Shukla, Shriyaa Mittal</i>	
<b>(508g) Deep Learning and Atomistic Simulations in High-Throughput Material Discovery .....</b>	259
<i>Amir Barati Farimani</i>	
<b>(508h) Advancing Molecular Simulation Methods with Machine Learning.....</b>	260
<i>Johannes Hachmann</i>	
<b>(537b) Saddle Point Searches in Electrochemical Reactions.....</b>	261
<i>Per Lindgren, Georg Kastlunger, Muammar El Khatib, Andrew A. Peterson</i>	
<b>(537d) Enhanced Activity for Oxygen Reduction Reaction By Gold at Step/Edge Sites of Ni@Aupt Core-Shell Nanoparticles: A DFT Investigation .....</b>	262
<i>Wei An, Hao Wang</i>	
<b>(537f) Ammonia Synthesis Using Plasma Assisted Catalysis: Understanding Rate Enhancements By Excited Species.....</b>	263
<i>Prateek Mehta, Jongseok Kim, David Go, Jason C. Hicks, William F. Schneider</i>	
<b>(551a) Systematic Multiscale Models and Physics Using the Relative Entropy.....</b>	264
<i>M. Scott Shell</i>	
<b>(551b) Development of a Top-Down Coarse-Grained Model for Protein Assemblies.....</b>	265
<i>Jeetain Mittal</i>	
<b>(551c) Accessing the Inaccessible: Studying the Liquid-to-Solid Transition in Molecular Simulations.....</b>	266
<i>Sapna Sarupria</i>	

<b>(551d) A Brief History of Exploring Hypothetical Crystal Structures</b>	267
<i>Christopher E. Wilmer</i>	
<b>(551e) Molecular Modeling of Adsorption of CO<sub>2</sub> and Water in Hydrophobic Metal-Organic Frameworks</b>	268
<i>Randall Q. Snurr, Peyman Z. Moghadam, Hongda Zhang</i>	
<b>(595a) Progress Towards Ultra-Fast Screening of Porous Sorbents for Chemical Separations</b>	269
<i>David S. Sholl, Dai Tang</i>	
<b>(595b) Identifying New Descriptors for Gas Storage in Nanoporous Materials</b>	270
<i>Benjamin Bucior, N. Scott Bobbitt, Arun Gopalan, Randall Q. Snurr</i>	
<b>(595c) Discovery of High-Performing MOFs Via Machine Learning</b>	271
<i>Alaaddin Ahmed, Donald J. Siegel</i>	
<b>(595d) Finding Truth in Fiction: Efficiently Discovering Physical Structure-Property Relationships By Screening Unphysical Porous Materials</b>	272
<i>Christopher E. Wilmer, Alec R. Kaja</i>	
<b>(595e) Mapping Transition Metal Chemical Space for Machine Learning Models</b>	273
<i>Jon Paul Janet, Heather J. Kulik</i>	
<b>(595f) Resolving 3D Structures of Metallic Nanoparticles from X-Ray Absorption Data Using Artificial Neural Network</b>	274
<i>Janis Timoshenko, Deyu Lu, Shinjae Yoo, Anatoly I. Frenkel</i>	
<b>(595g) Identifying Descriptors for Materials Science Via Genetic Programming: A Case Study for Dielectric Breakdown Strength</b>	275
<i>Fenglin Yuan, Tim Mueller</i>	
<b>(595h) Data-Driven Prediction of Materials Properties in an Automated Fashion</b>	276
<i>H. Shaun Kwak, Thomas J. L. Mustard, David J. Giesen, Thomas F. Hughes, Alexander Goldberg, Andrea R. Browning, Steve Dixon, Mathew D. Halls</i>	
<b>(595i) Computer-Aided Design of Novel Materials with Desired Electronic and Physical Properties</b>	277
<i>Olexandr Isayev</i>	
<b>(595j) Stability Prediction of Hypervalent Compounds Based on Data-Centric Modelling</b>	278
<i>Hans P. Luthi</i>	
<b>(595k) Human-Interpretable Reaction Informatics</b>	279
<i>Dmitry Zubarev</i>	
<b>(614a) Understanding the Removal of Pharmaceuticals from Water Effluents By Adsorption in Activated Carbons – A Molecular Simulation Approach</b>	280
<i>Lourdes F. Vega, Daniel Bahamon</i>	
<b>(614b) Insights into the Adsorption and Phase Behaviour of Fluids in Nanoporous Materials with Hierarchical Pore Structure: A Towards an Advanced Textural Characterization</b>	281
<i>Matthias Thommes</i>	
<b>(614c) Molecular Studies of Supercapacitors: Ionic Liquids Adsorbed into Porous Carbon Electrodes</b>	282
<i>Peter T. Cummings</i>	
<b>(614d) Structure of Ice in Confinement; Water in Mesopores</b>	283
<i>Malgorzata Sliwinska-Bartkowiak</i>	
<b>(614e) Towards Understanding the Role of Microstructure in Energetic Material Response: Coarse-Grain Modeling and Simulation</b>	284
<i>John K. Brennan</i>	
<b>(614g) Adsorption and Transport in Multiscale Porous Media</b>	285
<i>Benoit Coasne</i>	
<b>(656a) Developing Multi-Scale Models of Bimetallic Catalysts for the Hydrodeoxygenation of Bio-Oil Compounds</b>	286
<i>Breanna Wong, Greg Collinge, Alyssa Hensley, Yong Wang, Jean-Sabin McEwen</i>	
<b>(656b) Mechanistic Insights into Hydrodeoxygenation of Phenol on Bimetallic Phosphide Catalyst</b>	287
<i>Varsha Jain, Anna Taconi, Alicia Brown, Neeraj Rai</i>	
<b>(656d) Catalytic Conversion of Furfural to Methylfuran: Investigating Reaction Mechanisms on Ni and the Effect of Boron Doping on the Activity and Selectivity of the Catalyst</b>	288
<i>Arghya Banerjee, Samir H. Mushrif</i>	
<b>(656e) First-Principles Insights into the Mechanisms and Sites for Base Catalyzed Aldol Condensation and Esterification over Copper</b>	289
<i>Ashwin Chemburkar, Zhiyuan Tao, David D. Hibbitts, Enrique Iglesia, Matthew Neurock</i>	
<b>(656f) Advancing the Selective Oxidation of Ethylene Glycol Via Combining Novel Catalyst Design and Density Functional Theory (DFT) Calculations</b>	290
<i>Honghong Shi, Tuhin Suvra Khan, R. V. Chaudhari, M. Ali Haider, Bala Subramaniam</i>	

<b>(656g) Quantum Chemical Characterization of Catalytic Ester Decarbonylation: Olefins from Biomass.....</b>	291
<i>B. Dereli, Manuel Ortuno, Christopher Cramer</i>	
<b>(656h) Elucidating the Effect of External Electric Fields and Surface Dopants.....</b>	292
<i>Jacob Bray, Greg Collinge, Yong Wang, Catherine Stampfl, Jean-Sabin McEwen</i>	
<b>(675a) Uncovering Heterogeneous Ice Nucleation Using Advanced Molecular Simulations [Invited Talk].....</b>	293
<i>Sapna Sarupria, Brittany Glatz</i>	
<b>(675b) Investigation of the Chromatographic Separation of Chiral Drugs By Molecular Dynamics Simulation .....</b>	294
<i>Binwu Zhao, David W. House, Xiaoyu Wang, Priyanka Oroskar, Anil Oroskar, Asha Oroskar, Cynthia J. Jameson, Sohail Murad</i>	
<b>(675c) Molecular Simulation of CO<sub>2</sub> Absorption in Sorbent-Solvent Suspension and Interface Regions .....</b>	295
<i>Wei Shi, David Hopkinson</i>	
<b>(675d) Acid Gas Adsorption on Metal-Organic Framework Nanosheets As a Model of an "All-Surface" Material .....</b>	296
<i>Joshua Howe, Yang Liu, Luis Flores, David A. Dixon, David S. Sholl</i>	
<b>(675e) Contaminant Adsorption on <math>\text{Al}_2\text{O}_3</math>-Alumina Surface As Predicted By the Plane-Wave Density Functional Theory .....</b>	297
<i>Manoj Shukla</i>	
<b>(675f) Conformal Sites Model for Adsorbed Films on Energetically Heterogeneous Surface.....</b>	298
<i>Kaihang Shi, Erik E. Santiso, Keith E. Gubbins</i>	
<b>(675g) Identifying Relationships between Terminal Group Chemistry and Interfacial Friction in Monolayer-Based Lubrication through a Molecular Dynamics Screening Approach.....</b>	299
<i>Andrew Z. Summers, Christopher R. Iacovella, Peter T. Cummings, Clare McCabe</i>	
<b>(675h) Molecular Simulation Study of Aluminum <math>\text{\AA}</math> Noble Gas Interfacial Thermal Accommodation Coefficients.....</b>	300
<i>Haoyan Sha, Roland Faller</i>	
<b>(675i) The Water Flow through Graphene Slit Pores: Insights from Non-Equilibrium Molecular Dynamics Simulations .....</b>	301
<i>Mingjie Wei, Fang Xu, Yong Wang</i>	
<b>(685a) Enhanced Sampling Methods for Modulating Density Fields .....</b>	302
<i>Zhitong Jiang, Suruchi Fialoke, Amish Patel</i>	
<b>(685b) Mapped Averaging Methods for Accurate and Precise Evaluation of Free Energies and Other Properties By Molecular Simulation .....</b>	303
<i>Weisong Lin, Akshara Goyal, Sabry G. Moustafa, Andrew J. Schultz, David A. Kofke</i>	
<b>(685c) Predicting the Free Energy Landscape of Multicomponent Fluids.....</b>	304
<i>Nathan A. Mahynski, Jeffrey R. Errington, Vincent K. Shen</i>	
<b>(685d) A Novel Molecular Simulation Method for Liquid-Liquid Equilibria Predictions and in Silico Screening of Desalination Solvents .....</b>	305
<i>Prashanth Chandran, Jindal K. Shah</i>	
<b>(685e) Ssages: A Comprehensive Platform for Enhanced Sampling Simulations .....</b>	306
<i>Hythem Sidky, Yamil J. Colon, Benjamin J. Sikora, Cody Bezlik, Federico Giberti, Ashley Guo, Julian Helfferich, Xikai Jiang, Joshua Lequieu, Jiyuan Li, Joshua Moller, Michael Quevillon, Mohammad Rahimi, Hadi Ramezani-Dakhel, Vikramjit Rathee, Daniel Reid, Emre Sevgen, Vikram Thapar, Michael Webb, Justin Woźniak, Xujun Zhao, Nicola J. Ferrier, Olli G. Heinonen, Giulia Galli, Fran�ois Gygi, Juan J. De Pablo, Jonathan K. Whitmer</i>	
<b>(685f) Multiscale Modeling of Multicompartment Micelle Nanoreactors.....</b>	307
<i>Connor Callaway, Parveen Sood, Seung Soon Jang</i>	
<b>(685g) Reaction Ensemble Monte Carlo: Applications to Ionic Liquids .....</b>	308
<i>Ryan Gotchy Mullen, Edward J. Maginn</i>	
<b>(685h) Temperature-Dependent Physicochemical Properties of Nitrotoluenes from Solvation Free Energies .....</b>	309
<i>Alauddin Ahmed, Stanley I. Sandler</i>	
<b>(703a) Probing Topology and Reactant Effects on Hydride Transfer in Various Zeolites from First Principles .....</b>	310
<i>Thomas T. Chen, Matthew Neurock</i>	
<b>(703b) Simulations of Ammonia Adsorption for the Characterization of <math>\text{\AA}</math> Acid Sites in Metal-Doped Amorphous Silicates .....</b>	311
<i>Amy Jystad, Alessandro Biancardi, Marco Caricato</i>	
<b>(703c) First-Principles Grand-Canonical Simulations of Water Adsorption in Proton-Exchanged Zeolites Using a Highly Parallelizable Algorithm .....</b>	312
<i>Peng Bai, Matthew Neurock</i>	

<b>(703d) The Role of ABC-6 Zeolite Cavity in Methanol to Olefin Conversion.....</b>	313
<i>Xu Li, Jihong Yu, Jianwen Jiang</i>	
<b>(703e) Understanding the C-H Activation and Dehydrogenation Mechanisms of Alkanes on Metal Oxides .....</b>	314
<i>Mudit Dixit, Giannis Mpourmpakis</i>	
<b>(703f) Prediction and Screening of Product Distribution in Nanoporous Material-Catalyzed Propene Dimerization Via Molecular Simulations.....</b>	315
<i>Michelle Liu, Berend Smit</i>	
<b>(703g) Catalytic Hydrogenation of Carbon Dioxide in Functionalized Metal Organic Frameworks .....</b>	316
<i>Lin Li, Jingyun Ye, J. Karl Johnson</i>	
<b>(703h) Inorganometallic Catalyst Design: Alkane Metathesis Catalysis in Nu-1000 MOFs Functionalized with Transition Metals .....</b>	317
<i>Bo Yang, Kamal Sharkas, Laura Gagliardi, Donald G. Truhlar</i>	
<b>(736a) Automated Tests for Physical Validity in Molecular Dynamics and Monte Carlo Simulations .....</b>	318
<i>Pascal Merz, Michael Shirts</i>	
<b>(736c) Using Graphs to Quantify Energetic and Structural (dis)Order in Organic Thin Films .....</b>	319
<i>Alexander Hiller, Ellen Van, Matthew Jones, Eric Jankowski, Olga Wodo</i>	
<b>(736d) Interactive Extensible Molecular Simulations with Etomica .....</b>	320
<i>Andrew J. Schultz, Alexander D. Kofke, David A. Kofke</i>	
<b>(736e) A General Algorithm for Efficient Reverse-Mapping of Coarse-Grained Configurations to the Atomistic Scale.....</b>	321
<i>Christian Nowak, Mayank Misra, Fernando Escobedo</i>	
<b>(736f) Mosdef: Molecular Simulation and Design Framework.....</b>	322
<i>Christoph Klein, J. Sallai, Andrew Z. Summers, Christopher R. Iacobella, A. Ledeczi, Clare McCabe, Peter T. Cummings</i>	
<b>(736g) Massively-Parallel Mesoscale Hydrodynamics on Graphics Processing Units .....</b>	323
<i>Michael P. Howard, Athanassios Z. Panagiotopoulos, Arash Nikoubashman</i>	
<b>(736h) Foyer: A Framework for Defining Force Field Usage Semantics and Atom-Typing Molecular Systems .....</b>	324
<i>Christoph Klein, Andrew Z. Summers, Peter T. Cummings, J. Sallai, Christopher R. Iacobella, Clare McCabe</i>	
<b>(736i) Using the k-d Tree Data Structure to Accelerate Monte Carlo Simulations .....</b>	325
<i>Qile Chen, Bai Xue, J. Ilja Siepmann</i>	
<b>(747a) Machine Learning for Autonomous Crystal Structure Identification .....</b>	326
<i>Wesley F. Reinhart, Andrew W. Long, Michael P. Howard, Andrew L. Ferguson, Athanassios Z. Panagiotopoulos</i>	
<b>(747b) Intelligent, Autonomous Exploration of Self Assembly Simulation Parameter Space .....</b>	327
<i>Matthew Spellings, Sharon C. Glotzer</i>	
<b>(747c) Efficient Phase Diagram Sampling By Active Learning .....</b>	328
<i>Chengyu Dai, Isaac Bruss, Sharon C. Glotzer</i>	
<b>(747d) A Path Entropy-Based Approach to Predict Transition Rates from Limited Information .....</b>	329
<i>Purushottam Dixit</i>	
<b>(747e) Iterative Manifold Extension for Efficient Discovery of Transition Pathways .....</b>	330
<i>David Sroczynski, Juan Bello-Rivas, Hau-Tieng Wu, Eliodoro Chiavazzo, Ioannis G. Kevrekidis</i>	
<b>(747f) Learning Free Energy Landscapes Using Artificial Neural Networks .....</b>	331
<i>Hythem Sidky, Jonathan K. Whitmer</i>	
<b>(747g) QM/ML: A Hybrid Quantum-Mechanics/Machine-Learning Scheme.....</b>	332
<i>Yinjia Zhang, Andrew A. Peterson</i>	
<b>(747h) Automation of an Energy Renormalization Approach for the Temperature Transferable Coarse-Graining of Glass-Forming Polymers .....</b>	333
<i>Wenjie Xia, Brian Moroz, Jack F. Douglas, Sinan Keten, Frederick R. Phelan Jr.</i>	
<b>(747i) Developing Theory and Data-Driven Benchmarks for General Coarse-Grained Mapping Operators.....</b>	334
<i>Maghesree Chakraborty, Andrew White</i>	
<b>(747j) New Coarse-Grained Models of Hydrocarbons .....</b>	335
<i>Yixin An, Kartek K. Bejagam, Sanket Deshmukh</i>	
<b>(747k) Constrained Best Subset Selection Methodology for the Regression of Helmholtz Energy Equations .....</b>	336
<i>Marissa Engle, Nick Sahinidis</i>	
<b>(747l) Identifying Equilibrated Simulation Trajectories with Artificial Neural Networks .....</b>	337
<i>Eric Jankowski, Mitchell Leibowitz, Evan Miller, Michael Henry</i>	
<b>(773a) Deep Cavity Cavitand/Alkane Assembly State Switching between Monomeric and Dimeric Host:Guest Assemblies Driven By Guest Packing.....</b>	338
<i>Du Tang, J. Wesley Barnett, Bruce C. Gibb, Henry S. Ashbaugh</i>	

<b>(773b) Elucidating Protein (Folding) Kinetics Near Organic Surfaces As a Function of Surface Hydrophobicity .....</b>	345
<i>Elif Irem Senyurt, G. Zerze, Jeetain Mittal</i>	
<b>(773c) Serum Albumin Interactions with Doxorubicin-Loaded Graphene Oxide in an Aqueous Environment with Blood pH Level: A Molecular Dynamics Simulation Study .....</b>	346
<i>Mina Mahdavi, Sasan Nouranian, Ali Fattah</i>	
<b>(773d) Elucidating the Interaction Mechanisms of Thermo-Responsive Ligand with Proteins .....</b>	347
<i>Xiaoquan Sun, Xianghong Qian</i>	
<b>(773e) Study of Interaction and Transpassing of Human Beta Defensin-3 with Pops and Pops Membrane .....</b>	348
<i>Rabeta Yeasmin, Liqun Zhang</i>	
<b>(773f) Free Energy Calculation for Microcin J25 Variants Binding to the FhuA Receptor and to RNA Polymerase .....</b>	349
<i>Pin-Kuang Lai, Yiannis Kaznessis</i>	
<b>(773g) Predicting the Dimer Structure of Defensins Using a Combined Simulation Strategy .....</b>	360
<i>Liqun Zhang, Zhiming Feng, Aaron Weinberg</i>	
<b>(773h) Full-Atom Molecular Simulations of Lysozyme Confined in Realistic Silica Mesopores - Insights in Conformation and Accessibility of Active Sites .....</b>	361
<i>Katarzyna Maksimiak, Richard Catlow, Alberto Striolo, Marc-Olivier Coppens</i>	
<b>(773i) Aggregation and Self-Assembly of Biomimetic Polymers at Interfaces.....</b>	362
<i>Arushi Prakash, Christopher J. Mundy, Jim Pfaendtner</i>	
<b>Author Index</b>	