

Computational Molecular Science and Engineering Forum 2015

Core Programming Area at the 2015 AIChE Annual Meeting

Salt Lake City, Utah, USA
8-13 November 2015

ISBN: 978-1-5108-1855-2

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© (2015) by AIChE
All rights reserved.

Printed by Curran Associates, Inc. (2016)

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: 845-758-2634
Email: curran@proceedings.com
Web: www.proceedings.com

TABLE OF CONTENTS

(25a) A CFD Integrated Multiscale Method for Modeling Ethylene Oxidation Fixed Bed Reactors	1
<i>Behnam Partopour, Anthony G. Dixon</i>	
(25b) Multi-Scale CFD+Kmc Simulation of Methanol Partial Oxidation over Ceria in a Fixed Bed.....	2
<i>Qingang Xiong, Sreekanth Pannala, Stuart C. Daw, Aditya Savara, Steven H. Overbury</i>	
(25c) Analyzing and Compressing the Parametric Space for Modeling and Design of Heterogeneous Catalytic Systems	3
<i>Srinivas Rangarajan, Christos T. Maravelias, Manos Mavrikakis</i>	
(25d) Up-Scaling of Transport Processes in an Irregular Electrode Pore of a Lithium Ion Battery	4
<i>Njideka H. Okoye, Yung-Way Liu, Pedro E. Arce</i>	
(25e) Molecular Modeling of Pyrolysis Induced Shrinkage of Cellulose.....	5
<i>Abdul Salam Mohammad, Joseph J. Biernacki, Scott Northrup</i>	
(25f) Modeling of Diffusion and Catalytic Reactions of Gases in Highly Porous Nanolayers with Dsmc and Openfoam.....	6
<i>Georg R. Pesch, Norbert Riefler, Udo Fritsching, Lucio Colombi Ciacchi, Lutz Mädler</i>	
(25g) A Numerical Optimization Study on the Catalytic Dry Reforming of Methane in a Spatially Resolved Fixed-Bed Reactor	8
<i>Thomas Eppinger, Nico Jurtz, Ravindra Aglave, Gregor D. Wehinger, Matthias Kraume</i>	
(36f) Molecular-Dynamics-Assisted Molecular-Thermodynamic Framework to Predict the Interfacial Tensions of Non-Ionic Surfactants	10
<i>Vishnu Sresht, Daniel Blankschtein</i>	
(74a) Development of a Comprehensive Molecular Thermodynamic Model for High Salinity Produced Water in Oil and Gas Productions	11
<i>Chau-Chyun Chen</i>	
(74b) Gas Hydrate Phase Behavior in Presence of Organics and Electrolytes	12
<i>Cor J. Peters, Khalik Sabil</i>	
(74c) Phase-Portrait of Complex Kinetic Systems.....	13
<i>James Wei</i>	
(74d) Phase Equilibria of Ternary Mixtures of Two Nematic Liquid Crystals and CO2 for CO2 Capture	14
<i>Theo W. De Loos, Mariette De Groen, Thijs J. H. Vlugt</i>	
(74e) Effect of Additives on Hydrate Formation	15
<i>Jeong-Hoon Sa, Bo Ram Lee, Da-Hye Park, Gye-Hoon Kwak, Kunwoo Han, Kun-Hong Lee</i>	
(74f) Gas Hydrate Phase Equilibria at Extreme Conditions	27
<i>Amadeu K. Sum, Bo Ram Lee, Yue Hu</i>	
(74g) Thermodynamics in CO2 Capture By Chemical Absorption	28
<i>David Shan-Hill Wong, Meng-Ling Li</i>	
(74h) Representation and Validation of Liquid Densities for Pure Compounds and Mixtures	29
<i>John O'Connell, Vladimir V. Diky, Jens Abildskov, Kenneth Kroenlein, Michael Frenkel</i>	
(74i) Stanley Sandler's Contributions to the Development of Equations of State	32
<i>Arthur S. Gow</i>	
(76a) Sodium Octa-Vacancy Patterns in O3-NaMnO2 during Cycling.....	33
<i>Masoud Aryanpour, Young-Gyoon Ryu</i>	
(76b) The Crystal Structure of Coalescing Au and Its Alloy Nanoparticles By Ab Initio Molecular Dynamics	35
<i>Eirini Goudeli, Sotiris E. Pratsinis</i>	
(76c) Computational Screening of Metal-Ligand Systems for Methanol Carbonylation.....	36
<i>Nathan Duff, Erik E. Santiso</i>	
(76d) Liquid-Phase Mechanism Generation for Predicting Fuel Oxidation	37
<i>Belinda L. Slakman, Richard H. West</i>	
(76e) Force Field Optimization for Metal Oxide Fillers and Calculation of Mechanical and Thermal Properties of Epoxy-Based Composites	38
<i>David Rigby, Paul W. Saxe, Clive M. Freeman</i>	
(76f) Parameterizing Mosced with Molecular Simulation and Electronic Structure Calculations.....	52
<i>Andrew Paluch, Georgia Fuerst, Bryce Redeker, Ryan Ley, Jeremy Phifer</i>	
(76g) Prediction of the Solubility of Ethylene in Polyethylene Using Molecular Simulations at the Operating Conditions of LDPE Polymerization Process Equipment	53
<i>Sudheer Gondu, Jhumpa Adhikari</i>	

(145a) Development of a Molecular Model of Crude Oil: Applications in Enhanced Oil Recovery	54
<i>Nitish Nair, Kunj Tandon, Yusuf Kar, Hemalata Badiger, Marten Buijse, Johannes G. E. M. Fraaije, Jan-Willem Handgraaf</i>	
(145b) Rheological Study of Asphalt Using Molecular Simulation and Signal Processing	55
<i>Mohammad Masoori, Michael L. Greenfield</i>	
(145d) Molecular Simulation of Organic Electrolyte Solutions	56
<i>Maximilian Kohns, Steffen Reiser, Martin Horsch, Hans Hasse</i>	
(145e) Using Atomistic Simulation to Determine the Optimal Aggregation Number of a Micelle, and Its Equilibrium with Polymer Surface in Aqueous Solution	57
<i>Zifeng Li, Timothy Dipaolo, Kristen Fichthorn, Scott T. Milner</i>	
(145f) Pseudo Phase Diagrams of Supported Lipid Bilayers Formation: A Density Functional Theory Study	58
<i>Xian Kong, Diannan Lu, Jianzhong Wu, Zheng Liu</i>	
(145g) Prediction of Vapor and Sublimation Pressure for Pure Compounds from the Modified PR+Cosmosac Equation of State	59
<i>Li-Hsin Wang, Shiang-Tai Lin</i>	
(146a) Metal-Organic Frameworks for Liquid-Phase Applications: A Computational Perspective	60
<i>Jianwen Jiang</i>	
(146b) Modern Catalytic Technologies for Converting Biomass to Renewable Fuels and Chemicals	61
<i>Dionisios G. Vlachos</i>	
(146c) Molecular-Level Kinetic Modeling in Thermochemical Conversions: Software Tools and Their Applications	62
<i>Michael T. Klein</i>	
(146d) Simultaneous Determination of Liquid Dynamic Viscosity and Density of MEA and DEA Aqueous Solutions at Temperatures Between (313-353) K and Pressures up to 30 Mpa	63
<i>Luis A. Galicia-Luna, Jose J. Castro-Arellano, Alfredo Pimentel-Rodas</i>	
(146e) Ionic Liquids - Phase Behavior to Applications	64
<i>Mark Shiflett</i>	
(146f) Developing Quantum Mechanically-Based Force Field Parameters from Gas Hydrates to Biology	65
<i>Jeffery Klauda</i>	
(146g) Fundamentals and Applications of Antibody Solution Thermodynamics	66
<i>Peter M. Tessier</i>	
(146h) Thermodynamic Properties of Monoclonal Antibody Solutions	67
<i>Abraham M. Lenhoff</i>	
(146i) Multiscale Modeling for DNA Simulations	68
<i>Carol K. Hall, Emily Curtis, Abhishek Singh</i>	
(146j) Diffusion Coefficients of Carbon Dioxide in Liquid Hydrocarbons at High Pressures: Experiment and Modeling	69
<i>Shane Cadogan, Geoffrey Maitland, Bhavik Mistry, J. P. Martin Trusler, Y. Timothy Wong</i>	
(173a) Designing Software for Chemical Engineers – A Product Developer's Perspective	76
<i>Marco A. Satyro, Ross Taylor</i>	
(173b) Designing Chimeric Peptides Using Swarm Intelligence Optimization for the Protein Folding Problem	77
<i>Kyle Boone, Candan Tamerler, K. V. Camarda</i>	
(173c) A New Optimization Model for Computer-Aided Molecular Design Problems	78
<i>Lei Zhang, Stefano Cignitti, Rafiqul Gani</i>	
(173d) Designing Optimal Mixtures Using Generalized Disjunctive Programming: Convex Hull Reformulation	87
<i>Suela Jonuzaj, Claire S. Adjiman</i>	
(173e) A COSMO-Based Approach to Computer-Aided Mixture Design	88
<i>Nick Austin, Nick Sahinidis, Daniel W. Trahan</i>	
(173f) Coupling Experiments and Computational Tools to Estimate Thermal Properties for Product Design in the Fat-Based Food Industry	89
<i>Moises Teles Dos Santos, Icaro S. Viana, Juliana N. R. Ract, Galo A. C. Le Roux</i>	
(173g) Multi Objective Molecular Design of Reactants and Products	91
<i>Vikrant Dev, Nishanth G. Chemmangattuvalappil, Mario Richard Eden</i>	
(231a) Cheml- a Machine Learning and Informatics Program Suite for the Chemical and Materials Sciences	92
<i>Johannes Hachmann, Mojtaba Haghighatlari</i>	
(231b) A Molecular Workbench for Computational Soft Materials	93
<i>Frederick R. Phelan, Thomas Rosch, Cheol Jeong, Alden Dima, Mary Brady, Sharief Youssef</i>	

(231c) Mdn: A Web Portal for Network Analysis of Molecular Dynamics Simulations	94
<i>André A. S. T. Ribeiro, Vanessa Ortiz</i>	
(231d) Development of the Parallel Gibbs Ensemble Monte Carlo Simulation Engine Gomc	95
<i>Jason R. Mick, Loren Schwiebert, Brock Jackman, Kamel I. Rushaidat, Mohammad Barhaghi, Yuanzhe Li, Younes Nejahi, Jeffrey J. Potoff</i>	
(231e) Scalable Forward Flux Sampling, Scaffs: Enabling Large Scale Simulations of Rare Events	96
<i>Ryan Defever, Walter Hanger, Linh Ngo, Amy Apon, Sapna Sarupria</i>	
(247a) Oxidative Coupling of Methane: Descriptors for Activity and Selectivity	97
<i>Gaurav Kumar, Sai Lap Jacky Lau, Michael J. Janik</i>	
(247d) Entropic and Enthalpic Driving Forces on Morphology in Polymer Grafted Particle Filled Nanocomposites: Integral Equation Theory and Molecular Simulations	99
<i>Tyler B. Martin, Arthi Jayaraman</i>	
(247e) Hybrid Atomistic and Coarse-Grained Molecular Dynamics Simulations of Polyethylene Glycol (PEG) Chains in Explicit Water for Designing Peg Based Biomaterials	100
<i>Francesca Stanzione, Arthi Jayaraman</i>	
(247c) A New Lattice Monte-Carlo Simulation for the Dielectric Inhomogeneity of Ion-Containing Liquids	101
<i>Issei Nakamura, Xiaozheng Duan</i>	
(247f) Theoretical Investigation of Thermal Oxidation of Carbon-Coated Aluminum Nanoparticles Using the Reaxff Reactive Force Field	102
<i>Sungwook Hong, Adri Van Duin, Richard Yetter</i>	
(247b) The Effect of Halogenation of Erythrosine B on Amyloid-Beta 40 Oligomer Aggregation and Neurotoxicity in Alzheimer's Disease Using Molecular Modeling	103
<i>Hanbyeol Jin, Woo Yaa Lee, Sunju Kang, Jin Eun Shin, Joy Kim, Inchan Kwon, Seung Soon Jang</i>	
(247g) Exploring of the Pre-Polymerization Coordination of 1-Vinylimidazole	104
<i>J. Ryan Hamilton, Asghar Abedini, C. Heath Turner, John W. Whitley, Jason E. Bara</i>	
(247h) Local Hydration Structures and Dynamic Properties of Tetra-Alkyl Ammonium Aqueous Solution Systems: An Insight from Molecular Dynamics Simulations	105
<i>Dengpan Dong, Justin B. Hooper, Dmitry Bedrov</i>	
(247j) Insight into Selective Catalytic Reduction on Cu-SSZ-13 from Molecular Simulation	106
<i>Christopher Paolucci, Atish A. Parekh, Ishant Khurana, John R. Di Iorio, Hui Li, Trunojoyo Anggara, W. N. Delgass, Jeffrey T. Miller, Rajamani Gounder, Fabio H. Ribeiro, William F. Schneider</i>	
(247i) Assessment and Improvement of Methods for Computing Net Atomic Charges in Periodic and Nonperiodic Materials	107
<i>Nidia Gabaldon Limas, Thomas A. Manz</i>	
(247n) Molecular Dynamics Simulations of Mixtures of Refrigerants and Deep Eutectic Solvents	108
<i>Rubaiyet Abedin, Francisco R. Hung, John C. Flake</i>	
(247l) Molecular Modeling of Homogeneous Nucleation of [Bmim+][Cl-] from the Melt	109
<i>Yan Shen, Xiaoxia He, Francisco R. Hung, Erik E. Santiso</i>	
(247o) Equilibrium Properties of DNA Confined in Nanochannels: A Monte Carlo Chain Growth Approach	110
<i>Abhiram Muralidhar, Douglas R. Tree, Kevin D. Dorfman</i>	
(247p) The Mechanical Property of Dental Resin Composite Consisting of Bisgma and Tegdma Using Molecular Dynamics Simulations	111
<i>Jaeho Shin</i>	
(247q) Transport of Protein Shaped Colloids through Nanopores of Different Shapes	112
<i>Vincent Ustach, Roland Faller</i>	
(247r) Molecular Simulation of the Partitioning Phenomena of Oil and Dispersant Components in Air-Seawater-Oil System	113
<i>Zenghui Zhang, Thilanga Liyana-Arachchi, Paria Avij, Kalliat T. Valsaraj, Jennifer Field, Francisco R. Hung</i>	
(247t) Reaxff Reactive Molecular Dynamics Simulations with Explicit Electrons and Applications to Battery Interfaces	114
<i>Md Mahbulul Islam, Grigory Kolesov, Efthimios Kaxiras, Adri C. T. Van Duin</i>	
(247u) Developing Reaxff Force Field to Study Syngas Combustion Kinetics and Extending It for Larger Hydrocarbons	115
<i>Chowdhury Ashraf, Adri Van Duin</i>	
(247w) Molecular Dynamics Simulation of Lipid Bilayer Consisting of DPPC and Mppc: Effect of Configuration	116
<i>Young Kyoung Kim, Keewon Lee, Sang Eun Jee, Seung Soon Jang</i>	
(247y) Enhanced Oxygen Incorporation Near the Grain Boundary on Ytria-Stabilized Zirconia: A Density Functional Theory Study	117
<i>Kyeonghak Kim, Wonyoung Lee, Jeong Woo Han</i>	

(247z) Combining Spectroscopy Experiments and Molecular Simulation to Determine Structural and Mechanistic Details of Adsorbed Biomolecules	118
<i>Kayla Sprenger, Tobias Weidner, Jim Pfaendtner</i>	
(247x) Density Functional Theory Study of CO₂ Adsorption on Surface-Modified Graphene with Nitrogen Heterogeneity	119
<i>Geun Sik Lim, Ki Bong Lee, Hyung Chul Ham</i>	
(247aa) Microscopic Diffusion of CO₂ in Clay Nanopores.....	120
<i>Hassan Aljama, Chun-Yaung Lu, Jennifer Wilcox</i>	
(247m) Force Field Development of Chloroethenes	121
<i>Himanshu Goel, Neeraj Rai</i>	
(247ab) Mesostructured Self-Assembly of 12-Hydroxystearate in Organic Solvents.....	122
<i>Ryan Gordon, Cameron F. Abrams</i>	
(247ac) Online Tools for the Trappe Family of Force Fields	123
<i>Becky Eggimann, J. Ilja Siepmann</i>	
(247s) Rapid Computation of Thermodynamic Properties over a Large Multidimensional Space of Nonbonded Parameters.....	124
<i>Levi N. Naden, Michael R. Shirts</i>	
(247ae) Atomistic Simulations of Unfolded and Intrinsically Disordered Proteins	125
<i>Gul H. Zerze, Jeetain Mittal</i>	
(247ah) Molecular Dynamics Simulations Study of Poly(p-phenylene oxide) Based Polymer Membrane for Alkaline Fuel Cells	126
<i>Hongchao Pan, Justin B. Hooper, Dmitry Bedrov</i>	
(247ai) Coarse-Grained Thermodynamic Models for Self and Directed Assembly of Small Ensembles of Colloidal Particles.....	127
<i>Raghuram Thyagarajan, Dimitrios Maroudas, Michael A. Bevan, David Ford</i>	
(247af) Unraveling the Dissolution Mechanism of Crystalline Cellulose in Alkaline–Urea Solutions	128
<i>Pan Chen, Ahmed E. Ismail</i>	
(247ag) Insight into the Formation Mechanism of Dimethyl Oxalate By Using the DFT Method.....	129
<i>Lixia Ling, Maohong Fan, Baojun Wang</i>	
(247k) Mie Potentials for Phase Equilibria: Application to Ethers and Sulfides	130
<i>Mohammad Barhaghi, Jeffrey J. Potoff</i>	
(247ak) Self-Assembled Multilayer Stacking of Titanyl Phthalocyanines on Graphene Surface	131
<i>Lalitasri Ravavarapu, Pabitra Choudhury</i>	
(247ad) Artificial Neural Network Modeling of Alpha-Alkene Polymerization with Zirconocene/MAO Catalyst.....	132
<i>Nikhil Prakash</i>	
(247aj) Qnpr (Quantitative Nanostructure Property Relationship) Study for Describing Optical Properties of Plasmon Nanomaterials Using 3D Descriptors.....	133
<i>Shounak Datta, Robert Herring, Mario Richard Eden</i>	
(247al) Still Looking for the Magic Spot: Dispersing Modified Fe₂O₃ in Lamellar PS-PMMA Diblock Copolymer By Vapor-Annealing Deposition	134
<i>Paola Posocco, Yasmin Mohamed, Irati Barandiaran, Marina Zweyer, Giovanna Baldini, Erik Laurini, Maurizio Fermeglia, Galder Kortaberria, Sabrina Pricl</i>	
(316a) Diffusion Wavelet-Based Decompositions for Coarse-Graining of Polymer Chains	135
<i>Berend Christopher Rinderspacher, Jaydeep Bardhan, Ahmed E. Ismail</i>	
(316b) Atomistic Simulation of the Structure and Mechanics of Semicrystalline and Heterogeneous Polymer Systems	136
<i>Nikolaos Lempesis, Pieter In 'T. Veld, Greg C. Rutledge</i>	
(316c) Dissipative Particle Dynamics with Diffusion and Reaction: Application to Blood Clotting	137
<i>Bruce Caswell, Alireza Yazdani, Zhen Li, George Em Karniadakis</i>	
(316d) Accelerating Ring-Polymer Molecular Dynamics Simulation: A Parallel-Replica Dynamics Approach	138
<i>Chun-Yaung Lu, Arthur F. Voter, Danny Perez</i>	
(316e) Prion Protein Conformational Statistics Via on-the-Fly Free-Energy Parameterization.....	139
<i>Alexis Paz, Cameron F. Abrams</i>	
(316f) Protein Dynamics in the Unfolded State with Optimized All-Atom Protein Models	140
<i>Gul H. Zerze, Robert Best, Jeetain Mittal</i>	
(316g) An Integrated Framework Advancing Membrane Protein Modeling and Design.....	141
<i>Jeffrey J. Gray, Julia Koehler Leman, Rebecca Alford</i>	
(373a) Mapped Averaging: Reformulation of Ensemble Averages for High-Precision, High-Efficiency Calculation of Properties By Molecular Simulation	142
<i>Andrew J. Schultz, Sabry Moustafa, Weisong Lin, David A. Kofke</i>	

(373b) Multiscale from Molecular to Continuum: A Hybrid Simulation Method for Multicomponent Systems	143
<i>Nikolai D. Petsev, L. Gary Leal, M. Scott Shell</i>	
(373c) Entropic Depletion Interactions Between Anisotropic Particles Studied Using a Rigorous, Efficient and Parallelizable Monte Carlo Method	144
<i>Jens Glaser, Andrew Karas, Sharon C. Glotzer</i>	
(373d) Easy Transition Path Sampling in the Microcanonical Ensemble	145
<i>Ryan Gotchy Mullen, Joan-Emma Shea, Baron Peters</i>	
(373e) Incorporation of Chemical Equilibria into Dissipative Particle Dynamics.....	146
<i>Aleksey Vishnyakov, Ming-Tsung Lee, Alexander V. Neimark</i>	
(373f) Toward a New Generation of Reactive Force Fields: Polarizable Reactive Force Field (ReaxFP).....	147
<i>Saber Naserifar, Daniel Brooks, Vaclav Cvicek, Qingsong Zhang, William A. Goddard</i>	
(373g) Improving the Efficiency of Visited States Approaches to Expanded Ensemble Simulations	148
<i>Michael R. Shirts</i>	
(432a) Charge-Transfer Dynamics of Light-Harvesting Systems in Complex Solvated Environments	149
<i>Bryan Wong, M. Belen Oviedo</i>	
(432b) Computer Simulation of Nucleation of the Ionic Liquid [Dmim+][Cl-] in the Bulk and Near Graphitic Surfaces	150
<i>Xiaoxia He, Erik E. Santiso, Francisco R. Hung</i>	
(432c) A Statistical Approach to Reducing Finite-Size Effects from Gibbs Ensemble Monte Carlo Simulations for Predicting the Critical Point	151
<i>Richard A. Messerly, W. Vincent Wilding, Thomas A. Knotts</i>	
(432d) The Role of Water in the Growth of NaCl Crystals	162
<i>Mark Joswiak, Michael F. Doherty, Baron Peters</i>	
(432e) Core Level Shifts in Cu-Pd Alloys As a Function of Bulk Composition and Structure.....	163
<i>Jacob R. Boes, John R. Kitchin</i>	
(432f) Finite-Size Corrections to Electrolyte Chemical Potentials Calculated from Molecular Simulations	164
<i>Jeff P. Thompson, Isaac C. Sanchez</i>	
(432g) Rapid Characterization and Validity Quantum Isotope Effect Between Light and Heavy Water through Two-Phase Thermodynamics Model	165
<i>Li Yang, Kuan-Yu Yeh, Shiang-Tai Lin</i>	
(462a) Invited Talk: Data Mining and Machine Learning in Colloidal Science*	166
<i>Sharon C. Glotzer</i>	
(462b) Detecting the True Dimensionality of Complex Dynamical Systems Using Nonlinear Manifold Learning	167
<i>Carmeline Dsilva, Ronen Talmon, Ray M. Sehgal, Ronald Coifman, Ioannis G. Kevrekidis</i>	
(462c) Local-Environment-Based Distance Metric for Dimensionality Reduction in Colloidal Self-Assembly.....	168
<i>Ray M. Sehgal, Michael A. Bevan, David Ford, Dimitrios Maroudas</i>	
(462d) Near Perfect Prediction of HIV-1 Coreceptor Usage Reveals the Interactions Driving Tropism	169
<i>Chris A. Kieslich, Phanourios Tamamis, Yannis A. Guzman, Melis Yildirim, Christodoulos A. Floudas</i>	
(462e) Creating an in silico Drug Discovery Pipeline for Faster Drug Discovery.....	170
<i>Jonathan J. Chen, Donald P. Visco</i>	
(462g) Qsars for Predicting Physicochemical and Biochemical Properties of Industrial Chemicals.....	188
<i>Dimosthenis Sarigiannis, Krystalia Papadaki, Periklis Kontoroupi, Spyros Karakitsios</i>	
(462h) Statistical Approaches to Crystal Engineering.....	190
<i>Philip Adler, Simon Coles, Lucy Mapp, Terry Threlfall, Dave Woods</i>	
(484a) Understanding Protein Transport in Polymer-Grafted Ion Exchangers through Multi-Scale Modeling.....	191
<i>Joseph Basconi, Michael R. Shirts, Giorgio Carta</i>	
(484b) Role of Protein Sequence in Driving Molecular Interactions Between Proteins and Carbon Nanomaterials: A Molecular Dynamics Study	192
<i>Siva Dasetty, Sapna Sarupria</i>	
(484c) Energy Network Analysis to Quantify Effects of Nanotubes on DNA/Peptide Strength of Interaction	193
<i>André A. S. T. Ribeiro, Vanessa Ortiz</i>	
(484d) The Role of DNA Sequence in Nucleosome Positioning and Sliding.....	194
<i>Joshua Lequeieu, Juan J. De Pablo</i>	
(484e) Conformational Thermodynamics of DNA Strands within Electrically Charged Nanopores	195
<i>Fernando J. A. L. Cruz, José P. B. Mota</i>	

(484f) Molecular Modeling of Fibronectin Adsorption on Topographically Nanostructured Rutile	
(110) Surfaces.....	200
<i>Chunya Wu, Mingjun Chen, Chuangqiang Guo, Peter T. Cummings, Ting Zheng</i>	
(484g) Theoretical Insight into the Behavior of Bacteriocins in a Model Membrane Environment.....	210
<i>Panagiota Kyriakou, Yiannis N. Kaznessis</i>	
(484h) Unmasking the Mystery Base Employed By the T. Reesei Cel6A Cellulase.....	211
<i>Heather B. Mayes, Brandon C. Knott, Michael F. Crowley, Andreas W. Götz, Jerry Ståhlberg, Linda J. Broadbelt, Gregg T. Beckham</i>	
(484i) Modeling Chiral Recognition Between Amino Acids and Vaterite Surfaces	212
<i>Michael S. Pacella, Wenge Jiang, Dimitra Athanasiadou, Valentin Nelea, Hojatollah Vali, Robert M. Hazen, Marc D. McKee, Jeffrey Gray</i>	
(620f) Toward Structure Prediction and Design of Protein Glycosylation	213
<i>Jeffrey J. Gray, Jason Labonte</i>	
(553c) Multiscale Simulations Can Reveal the Effect of Ionic Liquids on Structure and Dynamics of Biomolecules.....	214
<i>Jim Pfaendtner</i>	
(553d) Computer Simulations in the Massively Parallel Era and Beyond.....	215
<i>Joshua A. Anderson</i>	
(553e) Entropic Control over Nanoscale Colloidal Crystals.....	216
<i>Athanassios Z. Panagiotopoulos</i>	
(582a) Invited Talk: Materials Cartography- Mapping Chemical Design Pathways.....	217
<i>Krishna Rajan</i>	
(582b) Materials Informatics Platform for Property Prediction	218
<i>Olexandr Isayev</i>	
(582c) A Learning Framework to Accelerate First Principles Simulations	219
<i>Venkatesh Botu, Ramamurthy Ramprasad</i>	
(582d) Strategies for Efficiently Exploring Structure-Property Spaces Via High-Throughput Screening of Hypothetical Materials	220
<i>Alec Kaija, Christopher E. Wilmer</i>	
(582e) Application of a Genetic Algorithm to Screen Metal-Organic Frameworks: Pre-Combustion CO₂/H₂ Separation	221
<i>Yongchul G. Chung, Diego Gomez-Gualdrón, Peng Li, Nicolaas Vermeulen, Pravas Deria, Fraser Stoddart, Joseph T. Hupp, Omar K. Farha, Randall Q. Snurr</i>	
(582f) Computational Screening of MOFs with Open Metal Sites.....	222
<i>Emmanuel Haldoupis, Konstantinos D. Vogiatzis, Laura Gagliardi, J. Ilja Siepmann</i>	
(582g) Graph Based Technique to Quantify Charge Transport Characteristics of Heterogenous Morphologies.....	223
<i>Olga Wodo, Baskar Ganapathysubramanian</i>	
(582h) Deconstructing Detailed Reaction Mechanisms to Identify Species and Mine for Data	224
<i>Fariba Seyedzadeh Khanshan, Pierre L. Bhoorasingh, Belinda L. Slakman, Elliot H. Nash, Richard H. West</i>	
(631a) Molecular Theory for the Hydrophobic Interactions and Absorption of Span80 at a Squalane-Water Interface.....	225
<i>M. I. Chaudhari, Susan B. Rempe, D. Asthagiri, Liang Tan, Lawrence R. Pratt</i>	
(631b) Molecular Modeling of Select Organic Molecules at the Air-Water Interfaces.....	226
<i>Ojas Chaudhari, Joseph Biernacki, Scott Northrup</i>	
(631c) Molecular Dynamics Simulation of Amphiphilic Graphene Oxide As a Tunable Colloidal Surfactant in Oil/Water Mixtures	227
<i>Farzin Rahmani, Sasan Nouranian, Saeed Zajforoushan Moghaddam</i>	
(631d) Dynamics of Photo Switchable Patchy-Charged Surfaces.....	228
<i>Fateme Sadat Emami, Amir Vahid, Bartosz A. Grzybowski</i>	
(631e) Contact Charging Between Insulators: A Theoretical Study.....	229
<i>Xiaozhou Shen, Daniel J. Lacks</i>	
(631f) Solvent Effects on the Properties of Electric Double Layers with Surface Charge Regulation.....	230
<i>Dimitar N. Petsev, Mark Fleharty, Frank Van Swol</i>	
(631g) Multiscale Modeling of the Electrode/Electrolyte Interface Using Charge Optimized Many Body (COMB3) Potentials.....	231
<i>Sneha A. Akhade, Andrew Antony, Tao Liang, Michael J. Janik, Janna M. Maranas, Susan B. Sinnott</i>	
(631h) Surface Reaction, Solvent Inhomogeneity, and Ion Transport in Electric Double Layers: Predictions from a Classical Density Functional Theory	232
<i>Cheng Lian, Jianzhong Wu</i>	

(677a) Molecular Simulation of Adsorption and Separation of Pure Noble Gases and Noble Gas Mixtures on Single Wall Carbon Nanotubes	233
<i>Haoyan Sha, Roland Faller</i>	
(677b) Molecular Dynamic Simulation of Clay Particles Swelling	234
<i>Hassan Dashtian, Sahar Bakhshian, Yafan Yang, Muhammad Sahimi</i>	
(677c) Disruption of Ice Adhesion through Surface Functionalization	235
<i>Ben Schweitzer, Nick McDougall, Joseph Smith, Christopher Wohl, Richard Kreeger, Jose Palacios</i>	
(677d) Wetting and Interfacial Properties of CO₂/Brine/Illite System	249
<i>Chun-Yaung Lu, Jennifer Wilcox</i>	
(677e) Reactive Atomic Simulations of Kinetic Friction and Its Velocity Dependence at SiC/SiC Interfaces	250
<i>Nariman Piroozan, Saber Naserifar, Muhammad Sahimi</i>	
(677f) Interfacial Properties of Model Systems Using Isothermal Isobaric Monte Carlo Simulations.....	251
<i>Karnesh Jain, Jeffrey R. Errington</i>	
(677g) Characterizing the Curvature of Liquid-Vapor Interfaces and Its Effect on the Kelvin Equation Using Mean-Field Lattice Density Functional Theory	252
<i>Aaron Harrison, Stephen P. Beaudoin, David S. Corti</i>	
(677h) Molecular Dynamics Study of the Degradation of Alkylsilane Monolayers Under Shear	253
<i>Andrew Z. Summers, Christopher R. Iacovella, Matthew R. Billingsley, Steven T. Arnold, Peter T. Cummings, Clare McCabe</i>	
(677i) Thermodynamics of Cassie-Wenzel Transitions on Nanotextured Surfaces.....	254
<i>Amish Patel, Fnu Suruchi, Erte Xi</i>	
(723a) An Integrated Theoretical and Experimental Approach to the Design of Liquid Crystal-Based Chemical Sensors	255
<i>Luke T. Roling, Marco Bedolla, Sangwook Choi, Shixuan Fan, Robert Twieg, Nicholas L. Abbott, Manos Mavrikakis</i>	
(723b) Computational Design of MOF Arrays for Gas Sensing: Influence of Array Size on Sensor Performance	256
<i>Jenna Gustafson, Christopher E. Wilmer</i>	
(723c) Molecular Simulation of Proteins at Interfaces	257
<i>Jian Zhou</i>	
(723d) Partitioning of Organics into Surfactant Bilayers.....	258
<i>Rebecca K. Lindsey, Sumanth N. Jamadagni, David Eike, Peter Koenig, J. Ilja Siepmann</i>	
(723e) Adsorption and Electron Transfer of Bacterial Decaheme Cytochrome Mtrf on Gold Surface Studied with Atomistic Molecular Dynamics Simulation, Free Energy Computation and Kinetic Monte Carlo Simulation	259
<i>Heng Ma, C. Masato Nakano, Hye Suk Byun, Mohamed Y. El-Naggar, Tao Wei</i>	
(723f) Nanoparticle Interactions with Lipid Bilayer Studied with Ghost Tweezers Method	260
<i>Aleksey Vishnyakov, Sean Burgess, Alexander V. Neimark</i>	
(723g) Graphene Oxide Nanocarrier for Doxorubicin Anticancer Drug, a Molecular Dynamics Simulation Study.....	261
<i>Mina Mahdavi, Farzin Rahmani, Sasan Nouranian</i>	
(723h) DFT Calculations of Adlayer Structure of Tryptophan on Cu(111).....	269
<i>Rees B. Rankin</i>	
(723i) On the Requirements for the Formation and Shape of Precursors in Droplet Spreading	270
<i>Rolf E. Isele-Holder, Ahmed E. Ismail</i>	
(758a) Stability By Design (SbD): Utilizing Material Science Principles to Predict Physical and Chemical Stability of Pharmaceutical Solids.....	271
<i>Michael Brunsteiner, Corinna Gressl, Johannes G. Khinast, Amrit Paudel, Adrian L. Davis, Margaret Landis, Klimentina Pencheva, Garry Scrivens, Geoff Wood</i>	
(758b) Exploring Polymorph Free Energy Landscapes with Hamiltonian Reweighted Molecular Dynamics	274
<i>Eric Dybeck, Brittany Zimmerman, Natalie Schieber, Gerhard Koenig, Michael R. Shirts</i>	
(758c) Molecular Modeling to Design and Control (M2DC): A First Principles Approach to Polymorph Prediction and Crystallization Unit Design	275
<i>Conor Parks, Andy Koswara, Ramon Pena, Doraiswami Ramkrishna, Zoltan K. Nagy, Hsien-Hsin Tung, Shailendra Bordawekar</i>	
(758d) PAT for Form Monitoring during Drying	276
<i>Mina Dimitri</i>	
(758e) Molecular Modeling of Additive Effects on Calcium Pyrophosphate Crystals	277
<i>Nathan Duff, Chengxiang Liu, Erik E. Santiso</i>	
Author Index	