

Computational Molecular Science and Engineering Forum

Core Programming Topic at the 2012 AIChE Annual Meeting

**Pittsburgh, Pennsylvania, USA
28 October - 2 November 2012**

ISBN: 978-1-62276-721-2

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© (2012) by AIChE
All rights reserved.

Printed by Curran Associates, Inc. (2013)

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

AIChE
3 Park Avenue
New York, NY 10016-5991

Phone: (203) 702-7660
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

Modelling the Fluid Phase Behaviour of Aqueous Mixtures of Multifunctional Alkanolamines and Carbon Dioxide Using Transferable Parameters with the SAFT Approach	1
<i>Alexandros Chremos, Niall Mac Dowell, Javier Rodriguez, Felix Llovel, Amparo Galindo, Claire S. Adjiman, George Jackson</i>	
Molecular Simulations of Amine Functionalized MCM-41 for the Separation of CO₂/N₂	2
<i>Santiago Builes, Lourdes F. Vega</i>	
Process Model-Free Analysis of CO₂ Capture Systems	3
<i>John P. O'Connell, Nicholas McGregor, Jessie Kennedy, Paul M. Mathias</i>	
Electrochemically-Mediated Amine Regeneration for Carbon Dioxide Scrubbing Processes	4
<i>Michael C. Stern, Fritz Simeon, Howard Herzog, T. Alan Hatton</i>	
Dynamics Study and Gas Solubility in Phase Change Ionic Liquid for CO₂ Capture	5
<i>Hao Wu, Edward J. Maginn</i>	
Reversible Ionic Liquids for CO₂ Capture: A Thermodynamic Study	6
<i>Amy L. Rohan, Jackson R. Switzer, Kyle M. Flack, Emily C. Nixon, Amber C. Rumble, Elizabeth J. Biddinger, Manish Talreja, Pamela Pollet, Charles A. Eckert, Charles L. Liotta</i>	
Thermodynamic Model for CO₂ Absorption by Phase-Change Ionic Liquids	7
<i>Luke D. Simoni, Joan F. Brennecke, Mark A. Stadtherr</i>	
Molecular Simulation of Phase Equilibria and Self-Assembly: Progress and Challenges	8
<i>Athanassios Z. Panagiotopoulos</i>	
In-Pore Superhigh Pressure Effect On Solid Phase Transition and Organic Crystal Synthesis	9
<i>Koki Urita, Kozue Abe, Yuich Shiga, Tsutomu Itoh, Toshihiko Fujimori, Yoshiyuki Hattori, Tomonori Ohba, Takayoshi Arai, Kenji Hata, M. Yudasaka, S. Iijima, Isamu Moriguchi, Hirofumi Kanoh, Katsumi Kaneko</i>	
Isotropic-Polar Phase Transition in An Amphiphilic Fluid	12
<i>Martin Schoen</i>	
Insight Into Phase Behavior and Microstructure of Complex Fluids – in Honor of Keith Gubbins' 75th Birthday	13
<i>Walter G. Chapman, Bennett D. Marshall II, Kai Gong, Deepti Ballal, Kenneth R. Cox</i>	
Phase Transitions of Liquids Confined in Nano-Pores; The Novel Ice Structures	14
<i>Malgorzata Sliwinska-Bartkowiak</i>	
Nucleation From Solution: How Slow Diffusion Changes Everything	15
<i>Baron Peters</i>	
Molecular Modeling of Crystallization of Flexible Organic Molecules	16
<i>Erik E. Santiso, Andrei V. Kazantsev, Manolis Vasileiadis, Claire S. Adjiman, Constantinos C. Pantelides, Bernhardt L. Trout</i>	
Theoretical Calculating the Thermodynamic Properties of Solid Sorbents for CO₂ Capture Applications	17
<i>Yuhua Duan</i>	
Nonmonotonic Dependence of the Absolute Entropy On Temperature in Supercooled Stillinger-Weber Silicon	33
<i>Pankaj A. Apte, Arvind K. Gautam</i>	
Molecular Characterization of the Interactions of Growth Modifiers with Zeolite Surfaces	34
<i>Yogendra N. Pandey, Manolis Doxastakis</i>	
Efficient Monte Carlo Algorithms for Simulation of Crystalline Solids	35
<i>Andrew J. Schultz, David A. Kofke</i>	
GPU Accelerated Configurational Bias Monte Carlo Simulations of Linear Alkanes	36
<i>Jason R. Mick, Eyad Hailat, Vincent Russo, Kamel Ibrahim, Loren Schwiebert, Jeffrey J. Potoff</i>	
Estimating Physicochemical Properties of Amino Acid Side Chain Analogs Using Expanded Ensemble Molecular Simulation Algorithm: An Assessment of Force Fields	37
<i>Alauddin Ahmed, Stanley I. Sandler</i>	
Generating, Simulating, and Synthesizing Novel Materials for Gas Storage & Separations	38
<i>Christopher E. Wilmer, Omar K. Farha, Ki Chul Kim, Randall Snurr</i>	
Theoretical Investigation of the H₂ Oxidation On the Sr₂Fe_{1.5}Mo_{0.5}O_{6-d} (001) Perovskite Structure Under Anodic Solid Oxide Fuel Cell Conditions	39
<i>Suwit Suthirakun, Salai C. Ammal, Andreas Heyden</i>	
DFT Studies On Adsorption, Diffusion, and Clustering of Cu and Au On the Non-Polar ZnO(10-10) Surface	41
<i>Xiaowa Nie, Aravind Asthagiri</i>	
Mechanistic Analysis of the Selective Hydrogenation of Acetylene and Crotonaldehyde Over NiZn	42
<i>Jacob Held, Subhra Jana, Charles Spanjers, Michael Janik, Robert M. Rioux</i>	
Computational Modeling of Reconstruction Templated Adsorption On the Magnetite(001) Surface	43
<i>Thomas A. Manz, Gareth Parkinson, David S. Sholl, Ulrike Diebold</i>	
Poisoning Mechanisms of MgO-Supported Au Clusters in CO Oxidation	44
<i>Giannis Mpourmpakis, Michail Stamatakis, Nima Nikbin, Matthew A. Christiansen, Dionisios G. Vlachos</i>	
Quantum Dynamical Modeling of CO₂ Reduction Using Heterogenous Photocatalysis	45
<i>Chris Singer, Cynthia S. Lo</i>	
Mechanistic Study of CO Oxidation On Supported Gold Nanoparticles: How Nanoparticle Restructuring Impacts Reaction Energetics	46
<i>David A. Bruce, Ming He</i>	
Integrated Experimental and Computational Studies of Energy-Relevant Interfaces	47
<i>Peter T. Cummings</i>	

Interfacial Properties of Gas Hydrates in Energy Applications	48
<i>Carolyn A. Koh, Zachary M. Aman, E. Dendy Sloan, Amadeu K. Sum</i>	
CO₂/N₂ Separation in Metal Organic Framework Materials	49
<i>Perla B. Balbuena</i>	
From the Fundamentals of Porous Carbons Poromechanics to Applications for CO₂ Sequestration and Gas-Shale	50
<i>Roland J.-M. Pelleng, Laurent Brochard, Matthieu Van Damme, Franz-Josef Ulm</i>	
Combining Water, Argon and Nitrogen Adsorption for an Advanced Characterization of Ordered Nanoporous Carbons	51
<i>Matthias Thommes, Juergen Morell, Katie Cychosz, Michael Froeba</i>	
Modeling the Self-Assembly of Ordered Nanoporous Silica Materials	53
<i>Lin Jin, Scott M. Auerbach, Peter A. Monson</i>	
Understanding the Ion Exchange Properties in Zeolites From Monte Carlo Simulations	54
<i>Alain H. Fuchs</i>	
Monte Carlo On Gpus; A Proof of Detailed Balance	55
<i>Joshua A. Anderson, Eric Jankowski, Thomas Grubb, Michael Engel, Sharon C. Glotzer</i>	
Evaluating the Grand-Canonical Partition Function of Atomic and Molecular Fluids Using Expanded Wang-Landau Simulations	56
<i>Caroline Desgranges, Jerome Delhommelle</i>	
A Faster Simulation Method for Diffusion in Confinement	57
<i>Mahmoud Abouelnasr, Berend Smit</i>	
Development and Application of a Heuristic to Study Heterogeneous Nucleation Mechanisms	58
<i>Geoffrey P. F. Wood, Keith Chadwick, Erik E. Santiso, Bernhardt L. Trout</i>	
Computation of Entropic Effects in Crystal Structures	59
<i>Manolis Vasileiadis, Panagiotis (Panos) G. Karamertzanis, Claire S. Adjiman, Constantinos C. Pantelides</i>	
Molecular Density Functional Theory and Its Application to Hydration Free-Energy Calculations	60
<i>Shuangliang Zhao, Jia Fu, Jianzhong Wu</i>	
Multiscale Simulations of Curvature Inducing Protein Partitioning in the Presence of Mean and Gaussian Curvature Gradients	61
<i>Richard Tournet, Ryan P. Bradley, Natesan Ramakrishnan, Ravi Radhakrishnan</i>	
Exergy Analysis of Modular Organic Rankine Cycle (ORC) Power Plants	62
<i>Maciej Lukawski, Pall Valdimarsson, Jefferson W. Tester</i>	
Modeling Water Injected Gas Turbines - Performance and Emissions	63
<i>Mohammed Shafi Syed, Kerry M. Dooley, F. Carl Knopf</i>	
Injection of Carbon Dioxide and Nitrogen Into Methane Hydrate Reservoirs: Binary Hydrateressim Simulations	64
<i>Nagasree Garapati, Brian Anderson</i>	
Determination of Binary Parameters of Liquid-Liquid Equilibrium for Biodiesel + Glycerol + Ethanol Systems Using Local Composition Models	65
<i>Nathan Sombra, Frederico Do Carmo, Rilyvia Santiago-Aguiar, Hosiberto De Santxana</i>	
Regenerable MgO-Based Sorbents for CO₂ Removal in IGCC Processes	66
<i>Shahin Zarghami, Javad Abbasian</i>	
Hollow Fiber-Supported Designer Ionic Liquid Sponges for Post-Combustion CO₂ Scrubbing	67
<i>Jong Suk Lee, Patrick Hillsheim, Dongkun Huang, Ryan P. Lively, Kyung Hee Oh, Sheng Dai, William J. Koros</i>	
Prediction of CO₂ Adsorption Properties in Zeolites Using Force Fields Derived From Periodic Dispersion-Corrected DFT Calculations	68
<i>Hanjun Fang, Preeti Kamakoti, Ji Zang, Stephen Cundy, Charanjit Paur, Peter I. Ravikovitch, David S. Sholl</i>	
Structure Sensitivity of Dimethyl Ether Electro-Oxidation	69
<i>Jeffrey A. Herron, Luke Roling, Winny Budiman, Peter Ferrin, Manos Mavrikakis</i>	
Investigation of Ammonia Oxidation On the Platinum Surface for Hydrogen Generation	70
<i>Damilola A. Daramola, Gerardine G. Botte</i>	
Multiscale Modeling of the H₂ Oxidation Reaction At the Ni/YSZ Interface in the Presence and Absence of Sulfur	71
<i>Salai C. Ammal, Andreas Heyden</i>	
Effects of Crystal Structure, Oxidation State, Vacancy Concentration and Composition On Perovskite Reactivity	72
<i>John R. Kitchin</i>	
DFT Predictions On the Kinetics and Bond Selectivity of Propane Activation On Palladium Oxide(101) Surface	73
<i>Abbin Antony, Aravind Asthagiri, Jason F. Weaver</i>	
Modeling the Aldose- Ketose Isomerization by Lewis Acids in the Gas Phase and Aqueous Media. A Detailed Mechanistic Study	74
<i>Samir H. Mushrif, Stavros Caratzoulas, Vinit Choudhary, Stanley I. Sandler, Douglas J. Doren, Dionisios G. Vlachos</i>	
Direct Versus Hydrogen Assisted CO Dissociation On Metal Surfaces	75
<i>Dominic Alfonso</i>	
New Directions for Entropic Forces in Hard Particle Fluids	76
<i>Sharon C. Glotzer</i>	
A Pseudo-Quantum Description of Classical Vacancy Diffusion in Crystals	77
<i>Giovanni Ciccotti, Simone Meloni, Pierre-Antoine Geslin, Eric Vanden-Eijnden</i>	
2-Component Van Der Waals EoS and the Second Osmotic Virial Coefficient	78
<i>Benjamin Widom</i>	
Dissipative Particle Dynamics: Extensions and Emerging Applications	79
<i>John K. Brennan, Joshua D. Moore, Martin Lisal</i>	
Property Prediction with Analogous Series: A Continuum View of Discrete Molecular Entities	81
<i>Brian K. Peterson</i>	

SAFT-γ Coarse Grained Models for the Molecular Simulation of Complex Fluids with a Top-Down Methodology	82
<i>Carlos Avendano, Thomas Lafitte, Vassilis Papaionannou, Olga Lobanova, Claire Adjiman, Amparo Galindo, Erich A. Muller, George Jackson</i>	
Thermodynamic and Kinetic Models of the Emergence of Biological Homochirality	83
<i>Pablo G. Debenedetti, Harold W. Hatch, Frank H. Stilling, Francesco Ricci</i>	
Building a Better Pppm: Incorporating Long-Range Dispersion Interactions	84
<i>Rolf E. Isele-Holder, Paul S. Crozier, Ahmed E. Ismail</i>	
Precise Simulation of Fluid-Solid Transitions Using Constrained Cell Models	85
<i>Michael Nayhouse, Vincent R. Heng, G. Orkoulas</i>	
Obtaining the Contribution of Individual Atoms to the Energy and Stress Tensor From the Ewald and P3M Lattice Sum Methods	87
<i>Stan G. Moore, Timothy W. Sirk, Dean R. Wheeler, Eugene F. Brown</i>	
Parallel Tempering Metadynamics in the Well Tempered Ensemble: Getting More and Spending Less	88
<i>Jim Pfaendner, Michael Deighan, Max Bonomi</i>	
Identifying the Reaction Coordinate without Transition Paths: Dynamically Self-Consistent Projections	89
<i>Baron Peters, Peter Bolhuis, Ryan Gotchy Mullen, Joan-Emma Shea</i>	
On-the-Fly Free-Energy Parameterization Using Temperature-Accelerated MD	90
<i>Cameron F. Abrams, Eric Vanden-Eijnden</i>	
Using Multistate Reweighting to Rapidly Explore Molecular Parameter Space	91
<i>Himanshu Paliwal, Michael R. Shirts</i>	
Microscopic and Macroscopic Properties of Interfacial Water	92
<i>Tuan A. Ho, Raja Kirthi Kalluri, Dimitrios V. Papavassiliou, Alberto Striolo</i>	
An Asymptotically Consistent Approximant Method with Application to Soft and Hard-Sphere Fluids	93
<i>Nathaniel S. Barlow, Andrew J. Schultz, Steven J. Weinstein, David A. Kofke</i>	
CO₂-Induced Plasticization in Copolyimides Containing a Sulfone Group	94
<i>Sadiye Velioglu, M. Gökтуg Ahunbay, S. Birgül Tantekin-Ersolmaz</i>	
Molecular Dynamics Simulation Study of Tris(pentafluoroethyl)Trifluorophosphate-Based Ionic Liquid and Small Molecules Mixtures	96
<i>Xiaochun Zhang, Zhiping Liu, Xiaomin Liu, Suojiang Zhang</i>	
All-Atom and United-Atom Simulations of Guanidinium-Based Ionic Liquids	97
<i>Xiaomin Liu, Xiaochun Zhang, Xiaoqian Yao, Suojiang Zhang</i>	
Rational Design of DNA Functionalized Colloidal Particles	98
<i>Ian Jenkins</i>	
DFT Study of Structural, Electronic Properties and Acidity of TiO₂/USY	99
<i>Na Wang, Minhua Zhang, Yingzhe Yu</i>	
Two-Phase Thermodynamic Model for Efficient and Accurate Absolute Entropy of Water From Molecular Dynamics Simulations	100
<i>Pin-Kuang Lai, Shiang-Tai Lin</i>	
Molecular Simulations of Blends of Conjugated Polymers and Fullerene Derivatives for Bulk Heterojunction Organic Solar Cells	101
<i>Hilary S. Marsh, Arthi Jayaraman</i>	
Molecular Simulation Studies Relating Polycation Architecture to the Structure and Thermodynamics of Polycation-DNA Complexes	102
<i>Robert M. Elder, Arthi Jayaraman</i>	
Molecular Simulation Studies of Assembly of DNA-Grafted Nanoparticles: Effect of Grafted DNA Strand Sequence and Composition	103
<i>Arezou Seifpour, Steven R. Dahl, Arthi Jayaraman</i>	
Molecular Mechanisms for Self-Assembly in Neurodegenerative Diseases	104
<i>Erica A. Hicks, Caroline Desgranges, Jerome Delhommelle</i>	
Adsorption of Carbon Dioxide in Irmofs Using Molecular Simulations	105
<i>Jason M. Hicks, Caroline Desgranges, Jerome Delhommelle</i>	
Vapor-Liquid Equilibria Using Monte Carlo Wang-Landau Simulations	106
<i>Tsvetan Aleksandrov, Caroline Desgranges, Jerome Delhommelle</i>	
Towards More Efficient Enhanced Sampling Methods to Study Phase Transitions	107
<i>Kenneth N. Ngale, Caroline Desgranges, Jerome Delhommelle</i>	
Investigating β-Amyloid's Early Action On Hippocampal Neurons: A Computational Study	108
<i>Natasha P. Wilson, Theresa A. Good, Mariajose Castellanos</i>	
Molecular Modeling of the Ionic Liquid [EMIM+][TFMSI-] Inside a Slit Nanoporous Electrode: Effect of Charge Density, Pore Size and Pore Loading On Properties of Confined ILs	109
<i>Nav Nidhi Rajput, Joshua D. Monk, Ramesh Singh, Francisco R. Hung</i>	
Ionic Liquids Confined in Nanoporous Materials: Effects of Pore Size, Morphology and Material	110
<i>Ramesh Singh, Nav Nidhi Rajput, Joshua D. Monk, Francisco R. Hung</i>	
Toward a Systematic Coarse Grained Model of Phase Behavior in Assemblies of Colloidal Particles	111
<i>Ray M. Sehgal, David Ford, Dimitrios Maroudas</i>	
Ice Growth From Benzene, Naphthalene and Phenanthrene/Super-Cooled Water Solutions	112
<i>Thilanga P. Liyana-Arachchi, Kalliat T Valsaraj, Francisco R. Hung</i>	
Adsorption of Polar Compounds From Gas and Solution Phases Onto Zeolites	113
<i>Peng Bai, Michael Tsapatsis, J. Ilja Siepmann</i>	
Linear Basis Function Approaches to Efficient Free Energy Calculations	114
<i>Levi Naden, Tri T. Pham, Michael R. Shirts</i>	

Optimum Phase-Dependent Lennard-Jones Energy Cross-Parameters for Phase Equilibrium	115
<i>Suren Moodley, Kim Bolton, Deresh Ramjugernath</i>	
Probing the Adsorptive Behaviour of MIL-53(Al) Using Light Organics (C₁-C₄)	123
<i>Fernando J. A. L. Cruz, Andrey I. Lyubchik, Isabel A. A. C. Esteves, José P. B. Mota</i>	
Using Molecular Simulations to Understand Wetting of Fluid Mixtures	126
<i>Vaibhaw Kumar, Jeffrey R. Errington</i>	
Modeling Nonspecific Interactions in Biology	127
<i>Andrew D. White, Wenjun Huang, Ann K. Nowinski, Shaoyi Jiang</i>	
A Theoretical Study of the Hydration of Methane	128
<i>Alcione Garcia González, Daniel Porfirio Luis Jiménez, Humberto Saint-Martin</i>	
Simulations of Biomolecules in Nonaqueous Solvents	129
<i>Vance Jaeger, Jim Pfaendtner</i>	
GPU MCMC Developments: CBMC Nonpolar Molecules, Verlet Lists, and Architectural Optimizations	130
<i>Jason R. Mick, Kamel Ibrahim, Eyad Hailat, Vincent Russo, Loren Schwiebert, Jeffrey Potoff</i>	
New Methods for High Throughput Screening of Porous Materials	131
<i>Christopher E. Wilmer, Benjamin J. Sikora, Ki Chul Kim, Randall Snurr</i>	
Rapid Determination of Entropy and Free Energy of Mixtures From Molecular Dynamics Simulations with the Two-Phase Thermodynamic Model	132
<i>Pin-Kuang Lai, Shiang-Tai Lin</i>	
Slab-Based (SB) Ewald: An Efficient Lattice Sum Method for Lennard-Jones Fluids with 1-D Density Variations	133
<i>Stan G. Moore, Dean R. Wheeler</i>	
Enhanced Sampling of Peptide Adsorption and 2D Self-Assembly with Parallel Tempering Metadynamics [Invited Talk]	134
<i>Jim Pfaendtner, Michael Deighan</i>	
Lipid Self Assembly by Statistical Temperature Monte Carlo and Molecular Dynamics	135
<i>Lili Gai, Katie A. Maerzke, Christopher R. Iacovella, Clare McCabe, Peter T. Cummings</i>	
Programmable Self-Assembly of Nanoparticle Clusters Using DNA-Mediated Interactions	136
<i>Jonathan D. Halverson, Alexei V. Tkachenko</i>	
Simulation of Amyloid Beta in the Presence of Aggregation Inhibitors	137
<i>David C. Latshaw II, Carol K. Hall</i>	
Nanocubes and Nucleosomes: One Story of Assembly and Another of Disassembly [Invited]	138
<i>Gaurav Arya, Irina V. Dobrovolskaia, Bo Gao, Andrea Tao</i>	
Phase Behavior of Thermodynamically Small Assemblies of Colloidal Nanoparticles	139
<i>Ray M. Sehgal, Daniel J. Beltran-Villegas, Michael A. Bevan, Dimitrios Maroudas, David Ford</i>	
Disentangle Model Differences and Fluctuation Effects in DPD Simulations of Diblock Copolymers	140
<i>Qiang (David) Wang, Paramvir Sandhu, Delian Yang</i>	
Conversion of Hemicellulose to Furfural Using Solid Acid Catalysts in Gamma-Valerolactone, a Biomass-Derived Solvent	141
<i>James A. Dumesic, Elif I. Gurbuz, Stephanie G. Wettstein, David Martin Alonso</i>	
Insights Into the Selective Hydrogenation and Hydrogenolysis of Renewable Intermediates	142
<i>Matthew Neurock</i>	
Computational Methods for Exploring Reaction Paths in Catalytic Processes	143
<i>Martin Head-Gordon, Paul M. Zimmerman, Joseph S. Gomes, Shaama Mallikarjun Sharada, Alexis T. Bell</i>	
Sequential Quadratic Programming Framework for Ab Initio Structure Property Relationships in Amorphous Catalysts and Supports	144
<i>Bryan Goldsmith, Daniel Bean, Baron Peters</i>	
Computational Catalysis At Solid/Liquid Interfaces	145
<i>Andreas Heyden</i>	
Chemically Titrating Nucleation Sites On Oxide Surfaces with Fluorescent Probes	146
<i>Joseph M. McCrate, John G. Ekerdt</i>	
Making Nanostructures - New Views	147
<i>Alon V. McCormick</i>	
Using Computational Methods At Boeing to Solve Emerging Material Issues	148
<i>Kady Gregersen, Andrea R. Browning, Samuel Tucker, Stephen Christensen</i>	
Separation of Ethanol and Water: Molecular-Level Insights On Extraction and Adsorption Systems	149
<i>J. Ilja Siepmann, Samuel J. Keasler, Peng Bai</i>	
Solvation Free Energies and 1-Octanol/Water Partition Coefficients of Nitroaromatic Compounds Using Molecular Simulation Techniques	150
<i>Alauddin Ahmed, Stanley I. Sandler</i>	
Molecular Behavior of Water Confined in TiO₂ Nano-Slits Using Classical, Reactive and Ab Initio Molecular Dynamics	151
<i>Ming-Jie Wei, Peter T. Cummings</i>	
Fick Diffusion Coefficients In Ternary Liquids From Equilibrium Molecular Dynamics	152
<i>Xin Liu, Erin McGarrity, Ana Martin Calvo, Sofia Calero, Andre Bardow, Thijs Jh Vlugt</i>	
Using Molecular Simulations to Determine the Effective Permeabilities of Mixed Matrix Membranes of Polydimethylsiloxane with Increased Zeolite Loadings of Silicalite-1	153
<i>Paul F. Harten</i>	
Ethane/Ethylene Separation by Simulated Moving Bed: From Molecular Simulations to Process Design	154
<i>Miguel A. Granato, Vanessa F. D. Martins, João C. Dos Santos, Miguel Jorge, Alirio E. Rodrigues</i>	

Solvation Structure of Ions in Model Disordered Carbon Electrodes	155
<i>Katherine A. Phillips, Jeremy C. Palmer, Keith E. Gubbins</i>	
Catalytic Partial Oxidation of Methane On Platinum Investigated by Spatial Reactor Profiles, Spatially Resolved Spectroscopy, and Microkinetic Modeling	156
<i>Oliver Korup, Claude Franklin Goldsmith, Gisela Weinberg, Michael Geske, Timur Kandemir, Robert Schlögl, Raimund Horn</i>	
Multiscale Modeling of the Shock Compression of Energetic Materials Using Constant Energy Dissipative Particle Dynamics	157
<i>Joshua D. Moore, Sergei Izvekov, Martin Lisal, John K. Brennan</i>	
Efficient Catalyst-to-Reactor Methodologies for Novel Chemical Reactor Design and Scale-up	159
<i>Zbigniew Urban</i>	
Reaction-Diffusion Model of Multi-Component Parallel Reaction in Methanol Synthesis Catalyst and Optimization of the Size of Catalyst Particle	160
<i>Tao Li, Hui Han, Haitao Zhang, Dingye Fang, Weiyong Ying</i>	
A Multi-Scale Framework for CFD Modeling of Multi-Phase Complex Systems Based On the EMMS Approach	161
<i>Ning Yang, Jinghai Li</i>	
CFD Analysis of the Effect of Baffles On the Fluid Flow and Heat Transfer Inside the Shell of Cross-Flow Fixed Bed Reactor	166
<i>Yingzhe Yu, Yonghui Li, Lu Bai, Xiuqin Dong, Minhua Zhang</i>	
Modeling the Electrochemical Double Layer - CO₂ Reduction On Pt(111)	167
<i>Chuan Shi, Christopher O'Grady, Jens K. Norskov</i>	
Mechanistic Insights Into the Reduction of Nitric Oxide by Hydrogen On Platinum Catalysts	168
<i>Yunhai Bai, Carrie A. Farberow, Manos Mavrikakis</i>	
Development of Volcano Plots for Selected Reactions in Heterogeneous Catalysis and Electrocatalysis	169
<i>Rees B. Rankin, Jeff Greeley</i>	
Ab Initio Studies of Electron-Driven Photo-Reactions On Surfaces of Plasmonic Metal Nanoparticles	170
<i>Hongliang Xin, Marimuthu Andiappan, Phillip Christopher, Suljo Linic</i>	
First Principles Modeling of TiO₂ Rutile/Anatase Interfaces	171
<i>Juan Garcia, N. A. Deskins</i>	
First-Principles Investigation of H₂O Adsorption On Ti-Doped SnO₂(110) Surfaces	173
<i>Konstanze Hahn, Antonio Tricoli, Gianluca Santarossa, Angelo Vargas, Alfons Baiker</i>	
A First-Principles Study of Support Effects On the Adsorption of CO On Pt/SrTiO₃ (100)	177
<i>Simuck Yuk, Aravind Asthagiri</i>	
Thermodynamic and Kinetic Constraints On Viral Packaging [Invited]	178
<i>Michael F. Hagan</i>	
Thermodynamics of Protein-Mediated Self Assembly On Cell Membranes	179
<i>Natesan Ramakrishnan, Ravi Radhakrishnan</i>	
Monolayer and Electrode Geometry Effects On the Formation, Structure, and Conductance of Molecular Junctions	180
<i>William R. French, Christopher R. Iacovella, Peter T. Cummings</i>	
Inverse Design of Pairwise Interactions for Self-Assembly of Low-Coordinated Lattice Structures	181
<i>Avni Jain, Jeffrey R. Errington, Thomas M. Truskett</i>	
Packings and Self-Assembly of a Family of Hard Truncated Triangular Bipyramids	182
<i>Amir Haji-Akbari, Elizabeth R. Chen, Michael Engel, Sharon C. Glotzer</i>	
Self-Assembly of Grafted Nanoparticles in Thin Films	183
<i>Thomas Lafitte, Sanat K. Kumar, Athanassios Z. Panagiotopoulos</i>	
Computing Diffusivities in Spatially Periodic Media From the Rate Constants of Elementary Jumps Between Sorption Sites: Master Equation Solution by Recursive Reduction of Dimensionality	184
<i>Panagiotis D Kolokathis, Doros N. Theodorou</i>	
Bifurcation in Hexane Cracking On ZSM-5 and Faujasite Zeolites. A QM/MM/Qct Study	186
<i>Frerich J. Keil</i>	
Cs Promotion of the Reaction Rate for Gas Phase Epoxidation of Propylene Using H₂ and O₂ Over Au/TS-1	187
<i>W. Nicholas Delgass, Wen-Sheng Lee, M. Cem Akatay, Eric A. Stach, Fabio Ribeiro</i>	
Supported Molecular Catalysts: Characterization of the Metal and Metal-Support Interface Structures by Atomic-Resolution Transmission Electron Microscopy and Spectroscopy	188
<i>Jing Lu, Ceren Aydin, Nigel D. Browning, Bruce C. Gates</i>	
Immunology and Alex Bell	189
<i>Arup K. Chakraborty</i>	
Atmospheric Pressure Plasma Activation of Plastics for Improved Adhesion	190
<i>Robert F. Hicks, Thomas S. Williams, Hang Yu, Eleazar Gonzalez II</i>	
Boosting the Catalytic Performance of Complexes Confined in Mesopores by Controlling Pore Surface Curvature and Chemistry	191
<i>Marc-Olivier Coppens</i>	
On the Chemistry of Deformation: Theory of Solute Strengthening in Aluminum and Magnesium Alloys	192
<i>Louis Hector Jr.</i>	
Semi-Empirical AM1, PM3 and PM6 Calculations On the Metakaolin Molecular Structure: Practical Application in Geopolymer Cement Production	193
<i>Ojas Chaudhari, Joseph Biernacki, Scott Northrup</i>	
Theoretical and Experimental Studies of Water Absorption Into Ionic Liquids	195
<i>Wei Shi, David Luebke, Hunaid Nulwala, Krishnan Damodaran</i>	

Understanding Backbiting and Beta-Scission Reactions in Self-Initiated Polymerization of Methyl Acrylate: A Theoretical Study	196
<i>Shi Liu, Sriraj Srinivasan, Michael C. Grady, Masoud Soroush, Andrew M. Rappe</i>	
A Theoretical Study of Mechanisms for Chain Transfer to Monomer Reactions in Alkyl Acrylates	198
<i>Nazanin Moghadam, Masoud Soroush, Andrew M. Rappe, Shi Liu, Sriraj Srinivasan, Michael C. Grady</i>	
From Quantum Chemistry to Diesel Injector Deposits: Revisiting Liquid Phase Oxidation	200
<i>Amrit Jalan, Jorge Aguilera-Iparraguirre, Ionut M. Alecu, Joshua W. Allen, Caleb Class, Connie W. Gao, Gregory R. Magoon, Shamel S. Merchant, Richard H. West, William H. Green Jr.</i>	
Pathways of Liquefied Petroleum Gas Pyrolysis to Acetylene in Hydrogen Plasma: A Density Functional Theory Study	204
<i>Xiaoyuan Huang, Dang-Guo Cheng, Fengqiu Chen, Xiaoli Zhan</i>	
A Systematic Ab Initio Strategy for Predicting Structure-Activity Relationships of Catalysts On Amorphous Supports	203
<i>Bryan Goldsmith, Baron Peters</i>	
Initial Pathways to O Vacancy Formation On Pdo(101)	204
<i>Li Pan, Aravind Asthagiri</i>	
Newly Proposed Catalytic Route for the Production of Propylene Epoxide	205
<i>Thomas A. Manz</i>	
A DFT+U Investigation of Propene Oxidation Over Bismuth Molybdate	206
<i>Andrew (Bean) Getsoian, Vladimir Shapovalov, Alexis T. Bell</i>	
Developing Relationships for the Lewis-Catalyzed Alcohol Dehydration On Alumina	207
<i>Giannis Mpourmpakis, Dionisios G. Vlachos, Raymond J. Gorte</i>	
Theoretical Investigation of the Water-Gas Shift Reaction At the Three-Phase Boundary of Ceria (111) Supported Platinum Clusters	208
<i>Sara Aranifard, Salai C. Anmal, Andreas Heyden</i>	
A First-Principles Study On Carbon Dioxide Reforming of Methane Over Supported Pt Catalysts	209
<i>Zhuo Cheng, Vesna Havran, Nathan A. Fine, Brent Sherman, Cynthia S. Lo</i>	
Successful Applications of Molecular Modeling in Industry	N/A
<i>Mike Makowski, Jun Deng</i>	
A Reassessment of the Precision and Accuracy of Atomistic Calculations of Elastic Constants of Amorphous Engineering Polymer Glasses	210
<i>Paul W. Saxe, Clive M. Freeman, David Rigby</i>	
Understanding and Predicting Multimodal Ligand-Protein Interactions Using Molecular Simulations	211
<i>Siddharth Parimal, Melissa A. Holstein, Shekhar Garde, Steven M. Cramer</i>	
Coarse-Graining Protocol for Mesoscale Simulations of Nanostructured Polymers	212
<i>Aleksey Vishnyakov, Ming-Tsung Lee, Alexander V. Neimark</i>	
Ionic Effects On the Stability and Morphology of AOT-WATER-Isooctane Reverse Micelles: Molecular Dynamics and Dynamic LIGHT Scattering Perspective	213
<i>Victor R. Vasquez</i>	
The Investigation of Green Tea Catechin Binding to Keratins by Molecular Dynamics and Experimental Validation	214
<i>Jan Marzinek, Guoping Lian, Athanasios Mantalaris, Efstratios N. Pistikopoulos, Yanyan Zhao</i>	
Rational Platform for Biosurfactants Design Based On Molecular Dynamics and Experimental Validation Using Escherichia Coli Outer Membrane Protein A	215
<i>Angie Paola Macías, Diana Marcela Carrero Pinto, Nathalia Garces Ferreira, Harold Enrique Castro Barrera, Oscar A. Álvarez, Andrés Fernando González Barrios</i>	
Identifying Drug Binding Locations and Poses Using Hamiltonian Replica Exchange Molecular Dynamics	216
<i>Kai Wang, Michael R. Shirts, John D. Chodera</i>	
Many Integrated Core and the Coming Stampede: Intel Responds to the GPU	217
<i>Frank T. Willmore</i>	
GPU-Based High Performance Molecular Dynamics Simulation of Highly Heterogeneous Molecular Systems: Application for Three-Phase Model of Polymer Electrolyte Membrane Fuel Cell	218
<i>Ji Il Choi, Giuseppe F. Brunello, Seung Soon Jang</i>	
Optimization of a Lennard-Jones Particle Monte Carlo Gpucode	219
<i>Jason R. Mick, Eyad Hailat, Vincent Russo, Kamel Ibrahim, Loren Schwiebert, Jeffrey J. Potoff</i>	
GPU-Enabled Simulations of Size Effects On the Elongation and Rupture of Metallic Nanowires Using Many-Body Potentials	220
<i>William R. French, Christopher R. Iacovella, Peter T. Cummings</i>	
Adsorption of Atomic and Molecular Fluids in a Porous Material Using Expanded Wang-Landau Simulations	221
<i>Jerome Delhommelle, Caroline Desgranges</i>	
Adsorption of Carboxylate On Calcite (101 4) Surface: Molecular Dynamics Simulation Approach	222
<i>Byeongjae Chun, Seung Geol Lee, Giuseppe F. Brunello, Ji Il Choi, Seung Soon Jang</i>	
Mechanistic Studies of Chiral Recognition of Solutes by Amylose Tris[(S)-α-Methylbenzylcarbamate]	223
<i>Hung-Wei Tsui, Nien-Hwa Linda Wang, Elias I. Franses</i>	
Molecular Screening of Alcohol and Polyol Adsorption Onto MFI-Type Zeolites	224
<i>Ruichang Xiong, Stanley I. Sandler, Dionisios G. Vlachos</i>	
Molecular Simulation Studies of CO2 Adsorption From Mixtures of N2, CH4, and H2O by Microporous Carbon	225
<i>Yangyang Liu, Jennifer Wilcox</i>	
Pressure Enhancement in Nanopores: Effect of Pore Shape	226
<i>Yun Long, Keith E. Gubbins, Erich A. Muller, George Jackson, Erik E. Santiso</i>	

Exploring Solid-Fluid Phase Behavior of Adsorbed Water Nanoconfined Between Mica and Graphene Surfaces	227
<i>Cody K. Addington, Yun Long, Keith E. Gubbins</i>	
Engineering Entropy and Order in Nanomaterials Via Molecular Simulation	228
<i>Fernando Escobedo</i>	
Place Holder for Invited Plenary Speaker	229
<i>Juan J. Depablo</i>	
Linking Thermodynamics and Dynamics in Fluids: Re-Emergence of Excess Entropy Scalings for Transport Properties	230
<i>Thomas M. Truskett</i>	
Uncovering the Role of Water in Biomolecular Interactions	231
<i>Amish J. Patel, Patrick Varilly, Sumanth Jamadagni, David Chandler, Shekhar Garde</i>	
Simple Tests for Whether Simulation Data Is Consistent with the Desired Thermodynamic Ensemble	232
<i>Michael R. Shirts</i>	
Computational Spectroscopy of Protein Structure	233
<i>Yingying Jiang, Serdal Kirmizialtin Sr., Isaac C. Sanchez</i>	
Hydrogen Activation On Pt-Au Bimetallic Clusters: A DFT Study	234
<i>Minmin Hu, Douglas Linder, Marco Buongiorno Nardelli, Alberto Striolo</i>	
Lactic Acid Hydrogenation: DFT, Microkinetic Modeling and Experiments	235
<i>Suyash Singh, James A. Dumesic, Manos Mavrikakis</i>	
Reaction of Bio-Alcohols in H-FAU, H-Mor, H-ZSM-5 and H-ZSM-22	236
<i>Cuong Manh Nguyen, Marie-Françoise Reyniers, Guy B. Marin</i>	
Theoretical Insights Into the Effects of Hydrocarbon Structure On the Catalytic Hydrogenation of Unsaturated Ketones	243
<i>Bing Hao, Matthew Neurock</i>	
DFT and XANES Studies of d-Band Transition Metal Alloys	244
<i>Carolina Gomez, Tianpin Wu, Ruzica Todorovic, Neil Schweitzer, Jeffrey T. Miller, Randall Meyer</i>	
Establishing the Connection Between the Geometric and Electronic Structure of Oxygen Species On Ag Surfaces: First-Principles DFT and Monte Carlo Studies	245
<i>Matthew Morabito, Hongliang Xin, Suljo Linic</i>	
Factors Affecting the Catalytic Activation of the Carboxylate C-O-C Bond	246
<i>Ye Xu, Lijun Xu</i>	
Non-Equilibrium Surface Pattern Formation During Catalytic Reactions with Nanoscale Resolution	247
<i>Jean-Sabin McEwen, Pierre Gaspard, Thierry Visart De Bocarmé, Norbert Kruse</i>	
Morphological Studies of Conjugated Polymer Based Materials Using Coarse-Grained Molecular Simulations [Invited Talk]	248
<i>Arthi Jayaraman</i>	
Theoretical Calculations On Fullerene Derivatives	249
<i>Varuni Dantanarayana, Adam J. Moulé, Roland Faller</i>	
Heat Transfer Characteristics of a Nanofluid within a Heated Lid-Driven Cavity Using Multiscale Modeling Techniques	250
<i>John Shelton, C. F. Higgs III</i>	
Identification of Molecular-Level Contributions to Processivity in Glycoside Hydrolases From Computational and Experimental Studies of Serratia Marcescens Chitinases	251
<i>Christina M. Payne, Erik Kuhn, Gustav Vaaje-Kolstad, Vincent Eijsink, Morten Sørlie, Gregg T. Beckham</i>	
Multiscale Modeling of Cellulose Unzipping in Ionic Liquids	252
<i>Brooks D. Rabideau, Cesar Ojeda, Ahmed E. Ismail</i>	
Adsorption of Model Peptides and the Carbohydrate Binding Module: An Enhanced Sampling Molecular Dynamics Study	253
<i>Michael Deighan, Peter Englund, Jim Pfaendner</i>	
Free Energy of Desorption of Cello-Oligosaccharides From a Cellulose Crystal Surface	255
<i>Lakshmi Muthukumar, Rajesh Khare</i>	
First-Principles Characterization of Electronic Structure and Transport of e-/h+ Polaron Defects in Oxides: Application to TiO₂	256
<i>Michel Dupuis, N. A. Deskins, Roger Rousseau</i>	
First Principles Simulations of Siliceous Melts and Aggregating Vapors	257
<i>J. Ilja Siepmann, Kelly E. Anderson, Mohammadhasan Dinpajoo</i>	
Ab Initio Molecular Dynamics of Molecular Ions Contacting Carbon Nanotubes	258
<i>Wei Zhang, Lawrence R. Pratt, Gary Hoffman</i>	
Structure and Property of Glucose in DMSO/Water Mixtures From Ab Initio Molecular Dynamics Simulations	259
<i>Hongbo Du, Xianghong Qian</i>	
Probing the Growth of III/V Semiconductor Interfaces with Accelerated Rare-Event Simulations	260
<i>Yangzheng Lin, Kristen Fichthorn</i>	
First-Principles Simulations On High-Pressure Bonding Pathways for CO₂ Condensed Phases	261
<i>Anguang Hu</i>	
Influence of Sequence Distribution Effects On the Phase Behavior and Interfacial Properties of Random Copolymers	262
<i>Venkat Ganesan, Victor Pryamitsyn, Gunja Pandav</i>	
Modeling Solvent-Gradient Chromatography of Complex Polymers Using Statistical Theory of Interaction Polymer Chromatography	263
<i>Christopher J. Rasmussen, Yefim Brun, Brian McCauley, Alexander V. Neimark</i>	

Impact of Solvent Quality On the Hysteresis in the Coil-Stretch Transition of Flexible Polymers	264
<i>Rangarajan Radhakrishnan, Patrick T. Underhill</i>	
Atomistic Molecular Dynamics Simulations of Model Ionomers	265
<i>Dan S. Bolintineanu, Mark Stevens, Amalie L. Frischknecht</i>	
Stochastic Splitting Methods for Numerical Simulation of Rouse Chains in Flow	266
<i>Michael Howard, Scott Milner</i>	
Simulation of Polymer Crystal Growth with Various Morphologies Using a Phase-Field Model	267
<i>Mohsen Asle Zaeem, Sasan Nouranian, Mark F. Horstemeyer, Paul T. Wang</i>	
Reaction Coordinate for the Movement of Solvent Molecules in Glassy Amorphous Polymer	275
<i>Li Xi, Bernhardt L. Trout</i>	
Lipid Diversity: Is It Important in Modeling Organism and Organelle Membranes?	276
<i>Jeffery Klauda</i>	
Multiscale Modeling of Membrane Remodeling by the Protein Epsin	277
<i>Ryan P. Bradley, Ravi Radhakrishnan</i>	
Twisting Coarse-Grained DNA	279
<i>Margaret C. Linak, Kevin D. Dorfman</i>	
Predicting Anti-HIV-1 Activity of Tibo Compounds by QSAR Approach Using a New Topological Index	280
<i>Wang Qiang, Jia Qingchu, Ma Peisheng, Xia Shuqian, Tang Hongmei, Deng Yu</i>	
Understanding the Activation Mechanism of the Insulin Receptor Kinase Domain Using Enhanced Conformational Sampling and Free-Energy Calculations	287
<i>Harish Vashisth, Cameron F. Abrams</i>	
Free Energy Landscape of C Rugosa Lid Closing by Well-Tempered Metadynamics	288
<i>Patrick R. Burney, Jim Pfaendmer</i>	
Molecular Dynamics Study of Polymer Separation Using a Nanofluidic Staircase	289
<i>Frederick R. Phelan Jr., Christopher Forrey</i>	
Predictive Enzyme Catalysis and Protein Structure with Quantum Chemistry On GPUs	290
<i>Heather J. Kulik, Todd J. Martinez</i>	
Theoretical Insights On the Role of Defects in TiO₂ Surface Chemistry	291
<i>N. A. Deskins, Juan Garcia, Roger Rousseau, Igor Lyubinetsky, Michel Dupuis</i>	
Quantum Mechanical Study of Doping and Hydration Thermodynamics At the Surface of Yttrium-Doped Barium Cerate	292
<i>Tania A. Tauer, J. Will Medlin</i>	
Hopping Mechanisms in Dielectric Relaxation of Pyrochlores From First Principles Calculations	293
<i>Beverly Brooks Hinojosa, Aravind Asthagiri, Juan C. Nino</i>	
Density Functional Theory Calculations of the Interaction of Water with Forsterite (100) Surface	294
<i>Valentina Prigobbe, Dong-Hee Lim, Ana Suarez-Negreira, Jennifer Wilcox</i>	
An Ab Initio Equation of State for Supercritical Helium-4 Encapsulating Quantum Effects	297
<i>Katherine R. S. Shaul, Andrew J. Schultz, David A. Kofke</i>	
A Fermi-Liquid Theory for Electron Energy and Correlations	298
<i>Shuangliang Zhao, Jianzhong Wu</i>	
Understanding the Mechanisms of Cellulose Dissolution in Ionic Liquids	299
<i>Brooks D. Rabideau, Animesh Agarwal, Ahmed E. Ismail</i>	
Modeling Biomolecular Structure and Excitation Energy Transfer in Photosynthetic Pigment-Protein Complexes	300
<i>William P. Bricker, Linda N. Holyoke, Cynthia S. Lo</i>	
Polyelectrolyte Interactions At a Conducting Interface: A Simulation Study	301
<i>Maria Sammalkorpi, Paul Van Tassel</i>	
Molecular Dynamics Simulations of Thermoresponsive Poly (N-isopropylacrylamide) and Its Copolymer	302
<i>Hongbo Du, S. Ranil Wickramasinghe, Xianghong Qian</i>	
Molecular Simulation of Hydration of Zwitterion	303
<i>Qing Shao, Shaoyi Jiang</i>	
Structure of Rigid Hard-Ring Fluid	304
<i>Mariam Nouri, Marc Robert</i>	
Effects of Asphalt Compositions On Nanoscale Properties by Molecular Simulation	312
<i>Mohammad Masoori, Michael L. Greenfield</i>	
Toward a Molecular Model of SiC Nanoporous Membrane: Application of Reactive Molecular Dynamics Simulation to the Study of the Pyrolysis of Hpcs Polymeric Precursor	313
<i>Saber Naserifar, Lianchi Liu, Theodore T. Tsotsis, Muhammad Sahimi, William A. Goddard III</i>	
The 7th Industrial Fluid Properties Simulation Challenge	314
<i>Jonathan D. Moore</i>	
Author Index	