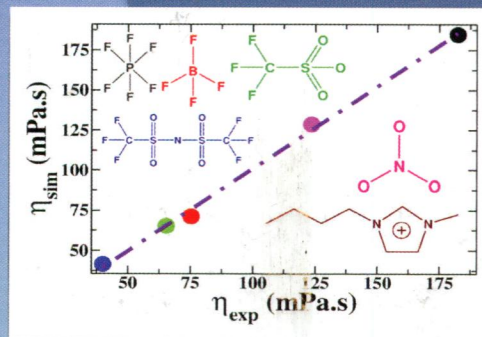
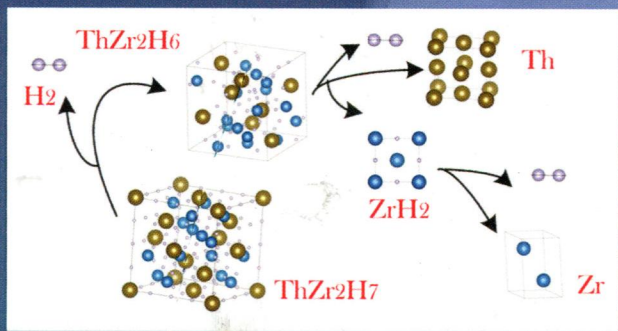
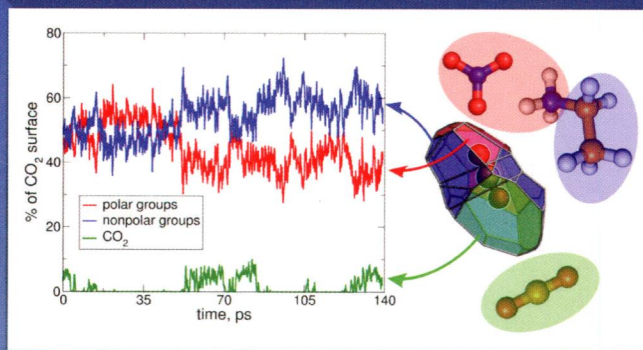
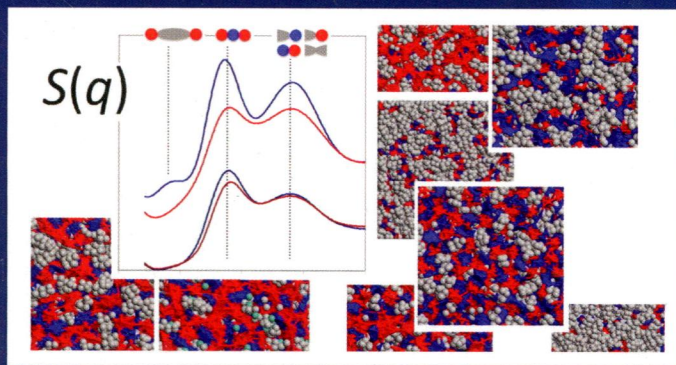


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**ON THE COVER:** The images shown on the cover were taken from papers in this special issue, Modeling and Simulation of Real Systems: (top) Experimental structure factor spectra of imidazolium-based ionic liquids with alkyl and glycol ether side chains and Molecular Dynamics simulation boxes of the studied ionic liquids. (see DOI: 10.1021/je500197x). (middle) Time development of the CO<sub>2</sub> surface covering by polar (the N', O", and H1 atoms) and nonpolar (the H2 and H3 atoms) groups, and other CO<sub>2</sub> molecules. (see DOI: 10.1021/je500166d). (left bottom) First-principles density functional theory and grand potential minimization methods are used to predict ternary interstitial hydride phase stability in the Th–Zr–H system (see DOI: 10.1021/je500250f). (right bottom) Comparison of computed and experimental shear viscosity values of room temperature 1-butyl-3-methylimidazolium cation-based ionic liquids. Computed values reproduce experimental data with remarkable accuracy (see DOI: 10.1021/je500132u).

## SPECIAL ISSUE: MODELING AND SIMULATION OF REAL SYSTEMS

### Editorial

2927

[dx.doi.org/10.1021/je500852y](http://dx.doi.org/10.1021/je500852y)

Foreword: Modeling and Simulation of Real Systems

Amparo Galindo

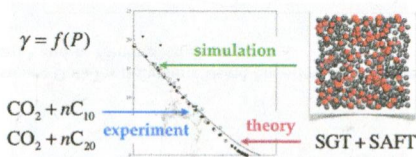
### Articles

2928

[dx.doi.org/10.1021/je5000764](http://dx.doi.org/10.1021/je5000764)

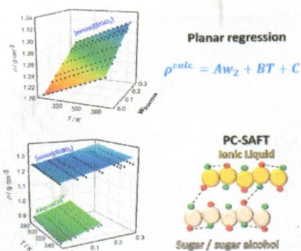
Use of Equations of State and Coarse Grained Simulations to Complement Experiments: Describing the Interfacial Properties of Carbon Dioxide + Decane and Carbon Dioxide + Eicosane Mixtures

Andrés Mejía,\* Marcela Cartes, Hugo Segura, and Erich A. Müller\*

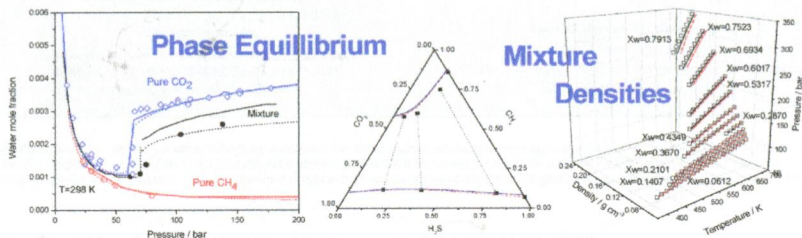


## Density of Mixtures Containing Sugars and Ionic Liquids: Experimental Data and PC-SAFT Modeling

Aristides P. Carneiro, Oscar Rodríguez, Christoph Held,\* Gabriele Sadowski, and Eugénia A. Macedo\*

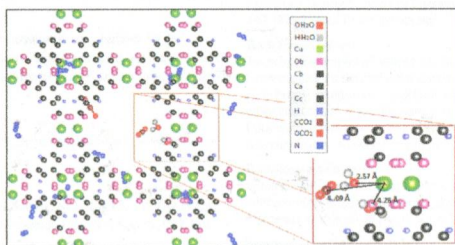
Modeling Phase Equilibria for Acid Gas Mixtures using the Cubic-Plus-Association Equation of State. 3. Applications Relevant to Liquid or Supercritical CO<sub>2</sub> Transport

Ioannis Tsvintzels,\* Shahid Ali, and Georgios M. Kontogeorgis



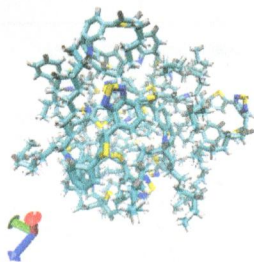
## Structure and Dynamics of Carbon Dioxide, Nitrogen, Water, and Their Mixtures in Metal Organic Frameworks

Hilda A. Mera, Jose L. Gomez-Ballesteros, and Perla B. Balbuena\*



## Molecular Dynamics Study of the Local Structure of Photovoltaic Polymer PCDTBT

Yusuke Kawanabe, Adam J. Moulé, and Roland Faller\*

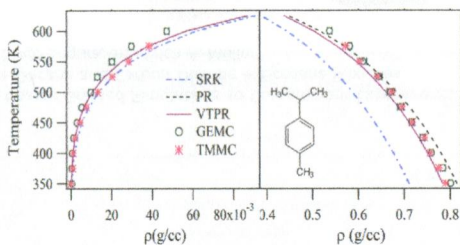


## 2987

dx.doi.org/10.1021/je5001022

Prediction of Vapor–Liquid Coexistence Data for *p*-Cymene Using Equation of State Methods and Monte Carlo Simulations

Madakashira Harini, Jhumpa Adhikari,\* and K. Yamuna Rani

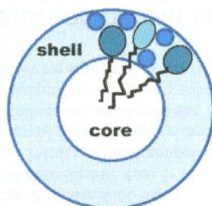


## 2995

dx.doi.org/10.1021/je500103h

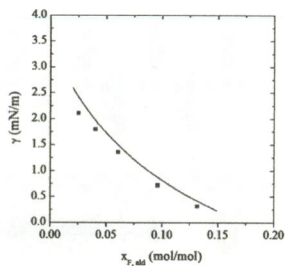
## Modeling of Micelle–Solution Equilibria for Mixed Nonionic Micelles with Strong Specific Interactions in Coronae: Group-Contribution Approach

Alexey I. Victorov\*



### Modeling of Liquid–Liquid Interfacial Properties of Binary and Ternary Mixtures

Elisabeth Schäfer, Franziska Horbach, and Sabine Enders\*

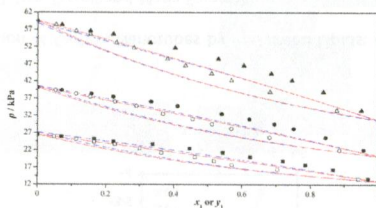


3017

dx.doi.org/10.1021/je500116z

### Phase Equilibrium of Binary Mixtures of *n*-Hexane + Branched Chlorobutanes: Experimental Results and Group Contribution Predictions

Victor Antón, M<sup>a</sup> Carmen Lopez, Beatriz Giner, and Carlos Lafuente\*

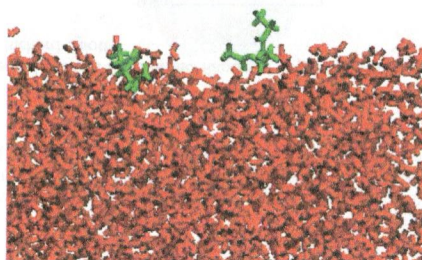


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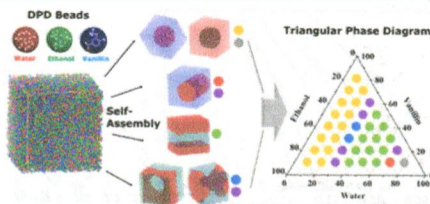
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### Green Leaf Volatiles on Atmospheric Air/Water Interfaces: A Combined Experimental and Molecular Simulation Study

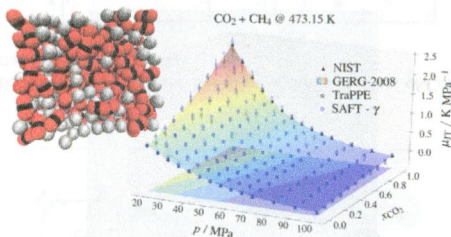
Thilanga P. Liyana-Arachchi, Zenghui Zhang, Harsha Vempati, Amie K. Hansel, Christopher Stevens, Andrew T. Pham, Franz S. Ehrenhauser, Kalliat T. Valsaraj, and Francisco R. Hung\*



Phase Behavior of Ternary Mixtures of Water–Vanillin–Ethanol for Vanillin Extraction via Dissipative Particle Dynamics  
Ga Eun Son, Nyambayar Sugartseren, Won-Byong Yoon, and Sang Kyu Kwak\*

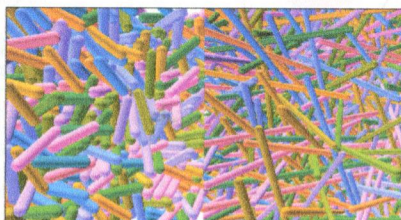


Thermodynamic Properties of Supercritical Mixtures of Carbon Dioxide and Methane: A Molecular Simulation Study  
Cassiano G. Aimoli, Edward J. Maginn,\* and Charles R. A. Breu



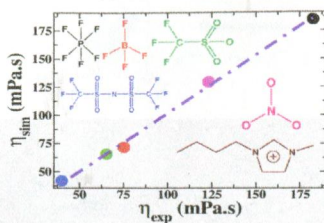
Random Packing of Hard Spherocylinders

Claudia Ferreiro-Córdova\* and Jeroen S. van Duijneveldt\*



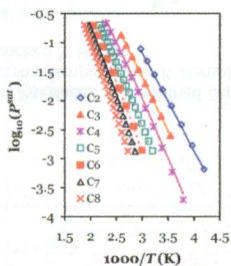
## A Molecular Dynamics Study of Collective Transport Properties of Imidazolium-Based Room-Temperature Ionic Liquids

Anirban Mondal and Sundaram Balasubramanian\*



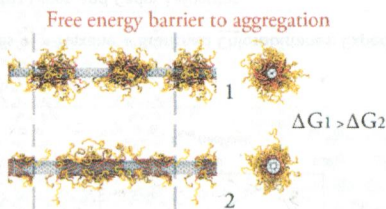
## Transferable Intermolecular Potential Models for a Broad Range of Organic Compounds

Amanda Sans, Amir Vahid, and J. Richard Elliott\*



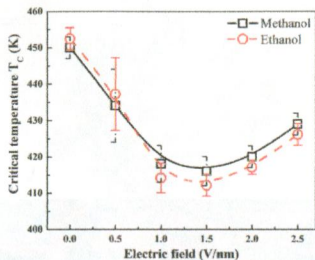
## Size-Selective, Noncovalent Dispersion of Carbon Nanotubes by PEGylated Lipids: A Coarse-Grained Molecular Dynamics Study

Jukka Määttä, Sampsa Vierros, Paul R. Van Tassel, and Maria Sammalkorpi\*

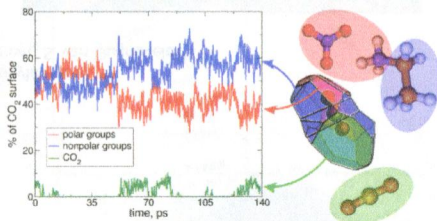


## Effects of Electric Field on the Vapor–Liquid Equilibria of Nanoconfined Methanol and Ethanol

Debdip Bhandary, Kartik Srivastava, Rajat Srivastava, and Jayant K. Singh\*

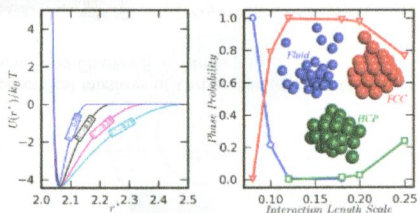
CO<sub>2</sub> Absorption in the Protic Ionic Liquid Ethylammonium Nitrate

Dzmitry S. Firaha and Barbara Kirchner\*



## Effects of the Attractive Potential Range on the Phase Behavior of Small Clusters of Colloidal Particles

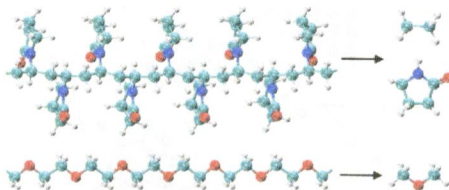
Ray M. Sehgal, Dimitrios Maroudas,\* and David M. Ford\*





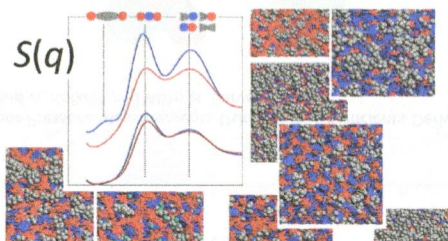
## Atomic-Scale Theory and Simulations for Colloidal Metal Nanocrystal Growth

Kristen A. Fichthorn\*



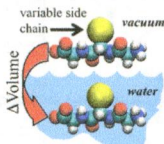
## Complex Structure of Ionic Liquids. Molecular Dynamics Studies with Different Cation–Anion Combinations

Adilson A. Freitas, Karina Shimizu,\* and José N. Canongia Lopes\*



## Direct Evaluation of Polypeptide Partial Molar Volumes in Water Using Molecular Dynamics Simulations

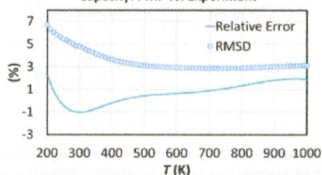
Lalitanand N. Surampudi and Henry S. Ashbaugh\*



## High-Throughput Calculations of Molecular Properties in the MedeA Environment: Accuracy of PM7 in Predicting Vibrational Frequencies, Ideal Gas Entropies, Heat Capacities, and Gibbs Free Energies of Organic Molecules

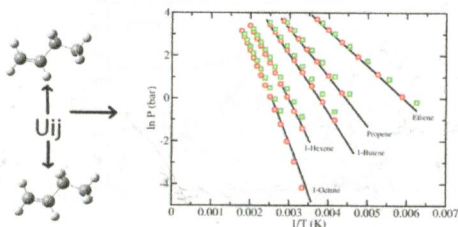
Xavier Rozanska,\* James J. P. Stewart,\* Philippe Ungerer, Benoit Leblanc, Clive Freeman, Paul Saxe, and Erich Wimmer

Evaluation of 160 Organic Molecules Heat Capacity: PM7 vs. Experiment



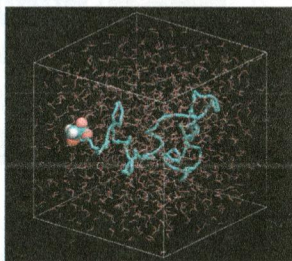
## Mie Potentials for Phase Equilibria: Application to Alkenes

Jeffrey J. Potoff\* and Ganesh Kamath



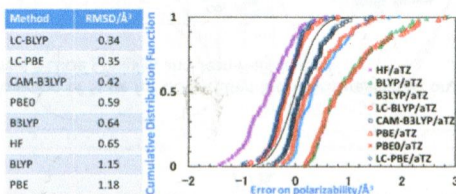
## Diffusion Coefficients of Fluorinated Surfactants in Water: Experimental Results and Prediction by Computer Simulation

Luís A. M. Pereira, Luís F. G. Martins,\* José R. Ascenso, Pedro Morgado, João P. Prates Ramalho, and Eduardo J. M. Filipe\*



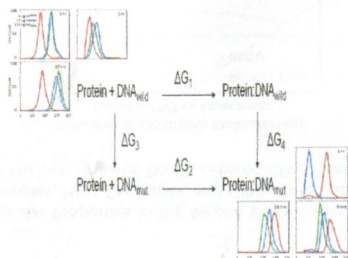
## Polarizabilities from Long-Range Corrected DFT Calculations

Shintaro Maekawa and Krzysztof Moorthi\*



## Investigation of Changes in Tetracycline Repressor Binding upon Mutations in the Tetracycline Operator

Dan S. Bolintineanu, Katherine Volzing, Victor Vivcharuk, Abdallah Sayyed-Ahmad, Poonam Srivastava, and Yiannis N. Kaznessis\*

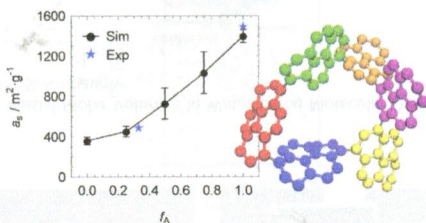


3177

dx.doi.org/10.1021/je5002329

## Porosity and Ring Formation in Conjugated Microporous Polymers

Lauren J. Abbott and Coray M. Colina\*

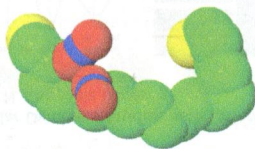


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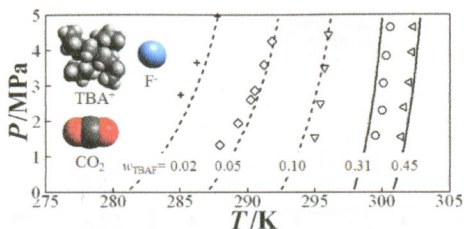
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## Interpreting Gas-Saturation Vapor-Pressure Measurements Using Virial Coefficients Derived from Molecular Models

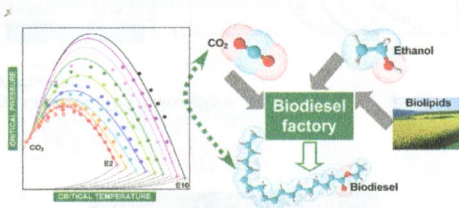
Shu Yang, Andrew J. Schultz, David A. Kofke,\* and Allan H. Harvey



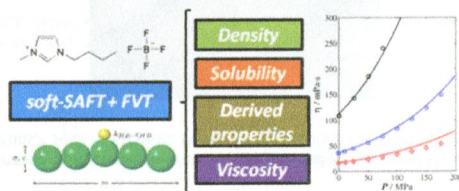
**Modeling the Dissociation Conditions of Carbon Dioxide + TBAB, TBAC, TBAF, and TBPB Semiclathrate Hydrates**  
 Ayako Fukumoto, Patrice Paricaud,\* Didier Dalmazzone, Wassila Bouchafaa, Thi Thu-Suong Ho, and Walter Fürst



**Development of a Predictive Equation of State for CO<sub>2</sub> + Ethyl Ester Mixtures Based on Critical Points Measurements**  
 Niramol Juntarachat, Romain Privat,\* Lucie Coniglio, and Jean-Noël Jaubert

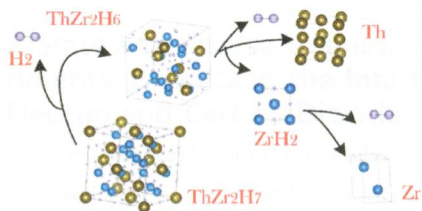


**Assessing Ionic Liquids Experimental Data Using Molecular Modeling: [C<sub>6</sub>mim][BF<sub>4</sub>] Case Study**  
 Felix Llovell\* and Lourdes F. Vega



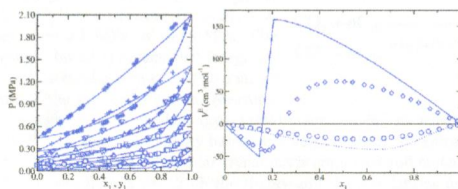
## First-Principles Prediction of Ternary Interstitial Hydride Phase Stability in the Th–Zr–H System

Kelly M. Nicholson and David S. Sholl\*

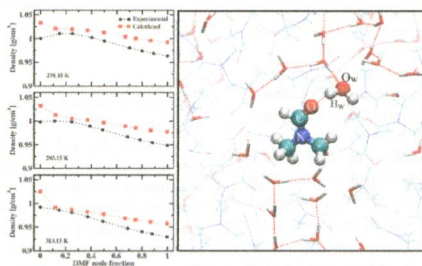


## Phase Equilibria and Excess Properties of Short-Alkane Mixtures Estimated Using the SAFT-VR Equation of State

Manuel M. Piñeiro,\* Felipe J. Blas, and María Carolina dos Ramos

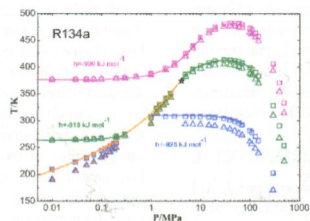
Effects of Temperature on the Structure and Dynamics of Aqueous Mixtures of *N,N*-Dimethylformamide

Sohag Biswas and Bhabani S. Mallik\*



## Molecular Simulation for Thermodynamic Properties and Process Modeling of Refrigerants

William R. Smith,\* Susana Figueroa-Gerstenmaier, and Magda Skvorova

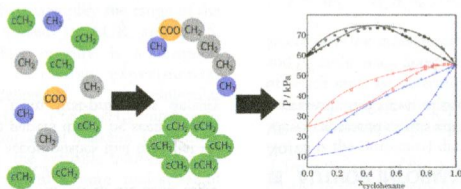


3272

dx.doi.org/10.1021/je500248h

Prediction of Thermodynamic Properties and Phase Behavior of Fluids and Mixtures with the SAFT- $\gamma$  Mie Group-Contribution Equation of State

Simon Dufal, Vasileios Papaioannou, Majid Sadeqzadeh, Thomas Pogiatzis, Alexandros Chremos, Claire S. Adjiman, George Jackson, and Amparo Galindo\*

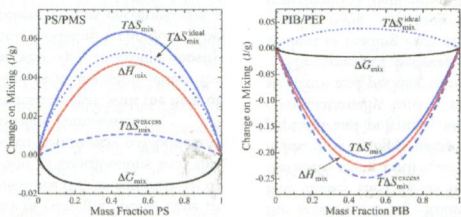


3289

dx.doi.org/10.1021/je5002818

## Connecting Theory and Experiment To Understand Miscibility in Polymer and Small Molecule Mixtures

Jane E. G. Lipson\* and Ronald P. White



# Prediction of Vapor–Liquid Coexistence Properties and Critical Points of Polychlorinated Biphenyls from Monte Carlo Simulations with the TraPPE–EH Force Field

Evgenii O. Fetisov and J. Ilja Siepmann\*

