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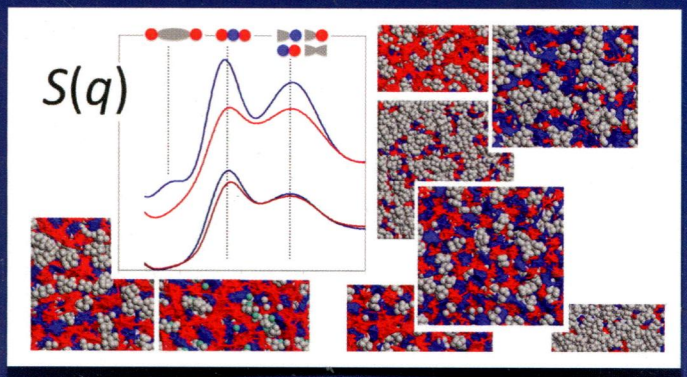

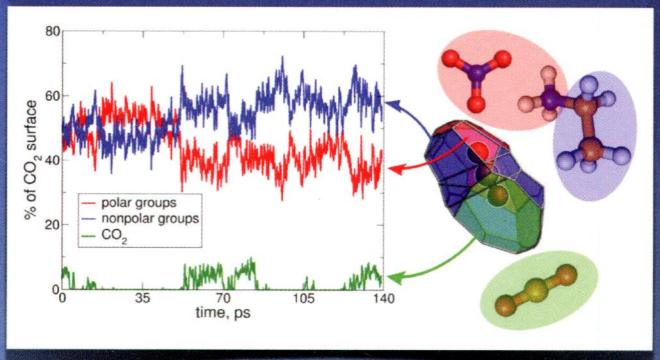

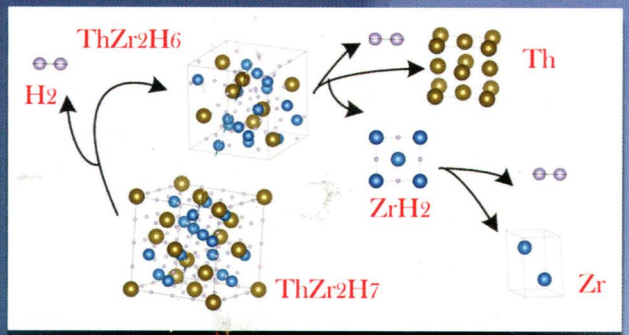

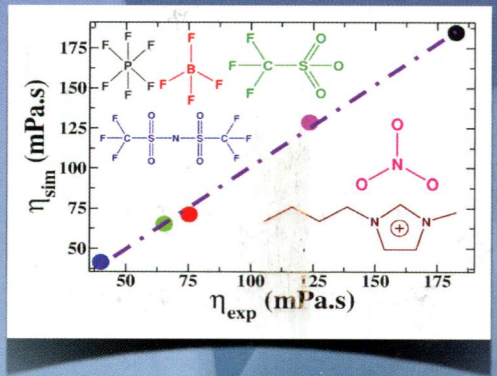

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Journal of chemical & engineering data

OCTOBER 2014
VOLUME 59 ISSUE 10

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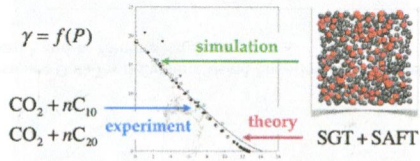
ON THE COVER: The images shown on the cover were taken from papers in this special issue, Modeling and Simulation of Real Systems: (top) Experimental structure factor spectra of imidazolium-based ionic liquids with alkyl and glycol ether side chains and Molecular Dynamics simulation boxes of the studied ionic liquids. (see DOI: 10.1021/je500197x). (middle) Time development of the CO_2 surface covering by polar (the N′, O″, and H1 atoms) and nonpolar (the H2 and H3 atoms) groups, and other CO_2 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 sheer 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

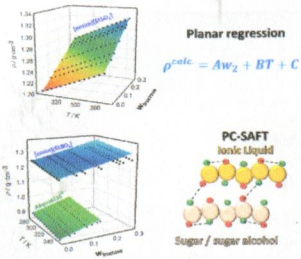
Articles



2942 dx.doi.org/10.1021/je500079y

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

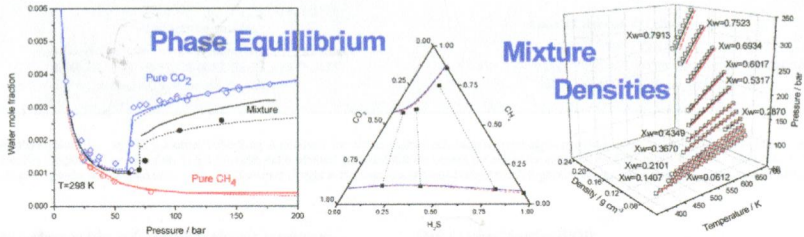
Aristides P. Carneiro, Oscar Rodríguez, Christoph Held,* Gabriele Sadowski, and Eugénia A. Macedo*



2955 dx.doi.org/10.1021/je500090q

Modeling Phase Equilibria for Acid Gas Mixtures using the Cubic-Plus-Association Equation of State. 3. Applications Relevant to Liquid or Supercritical CO_2 Transport

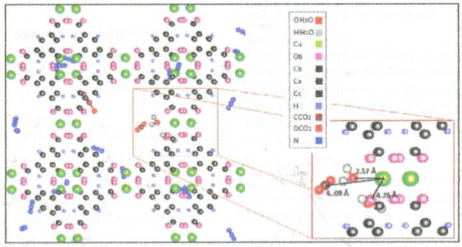
Ioannis Tsivintzelis,* Shahid Ali, and Georgios M. Kontogeorgis

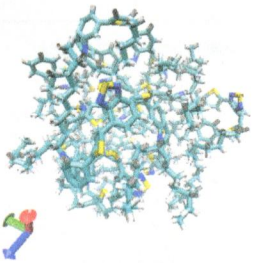


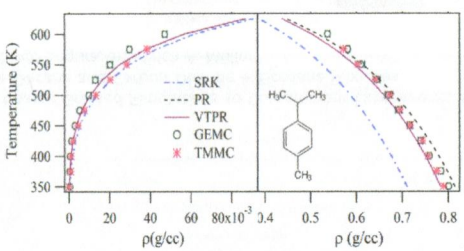
2973 S dx.doi.org/10.1021/je500100f

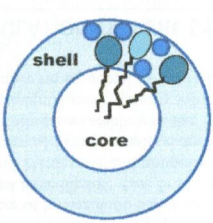
Structure and Dynamics of Carbon Dioxide, Nitrogen, Water, and Their Mixtures in Metal Organic Frameworks

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



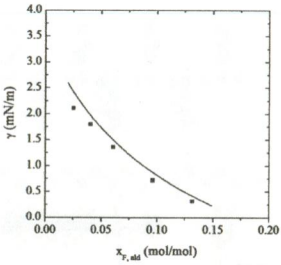






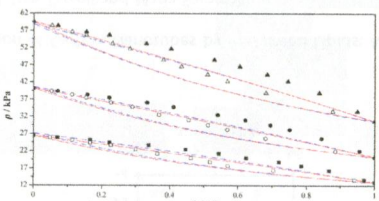
3003 dx.doi.org/10.1021/je500113q

Modeling of Liquid–Liquid Interfacial Properties of Binary and Ternary Mixtures
Elisabeth Schäfer, Franziska Horbach, and Sabine Enders*



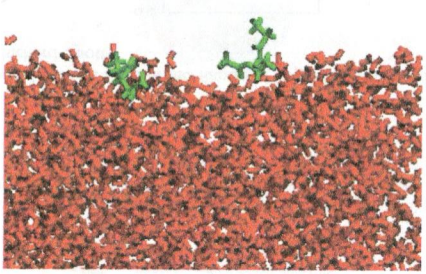
3017 S dx.doi.org/10.1021/je500116z

Phase Equilibrium of Binary Mixtures of *n*-Hexane + Branched Chlorobutanes: Experimental Results and Group Contribution Predictions
Victor Antón, M[a] Carmen Lopez, Beatriz Giner, and Carlos Lafuente*



3025 S dx.doi.org/10.1021/je500114m

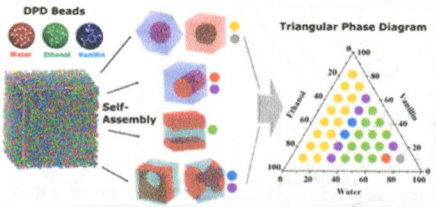
Green Leaf Volatiles on Atmospheric Air/Water Interfaces: A Combined Experimental and Molecular Simulation Study
Thilanga P. Liyana-Arachchi, Zenghui Zhang, Harsha Vempati, Amie K. Hansel, Christopher Stevens, Andrew T. Pham, Franz S. Ehrenhauser, Kalliat T. Valsaraj, and Francisco R. Hung*



3036 dx.doi.org/10.1021/je5001186

Phase Behavior of Ternary Mixtures of Water–Vanillin–Ethanol for Vanillin Extraction via Dissipative Particle Dynamics

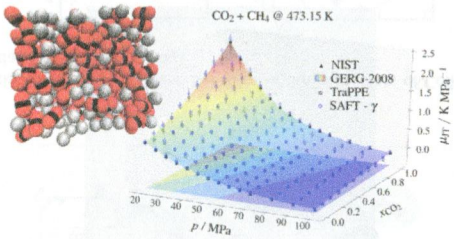
Ga Eun Son, Nyambayar Sugartseren, Won-Byong Yoon, and Sang Kyu Kwak*



3041 S dx.doi.org/10.1021/je500120v

Thermodynamic Properties of Supercritical Mixtures of Carbon Dioxide and Methane: A Molecular Simulation Study

Cassiano G. Aimoli, Edward J. Maginn,* and Charlles R. A. Abreu



3055 dx.doi.org/10.1021/je500119r

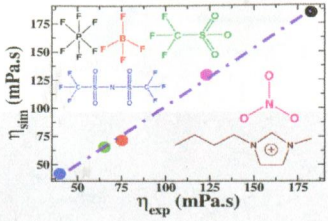
Random Packing of Hard Spherocylinders

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

3061 dx.doi.org/10.1021/je500132u

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

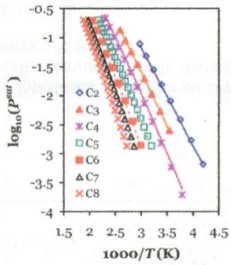
Anirban Mondal and Sundaram Balasubramanian*



3069 dx.doi.org/10.1021/je500151a

Transferable Intermolecular Potential Models for a Broad Range of Organic Compounds

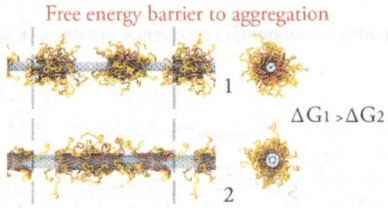
Amanda Sans, Amir Vahid, and J. Richard Elliott*

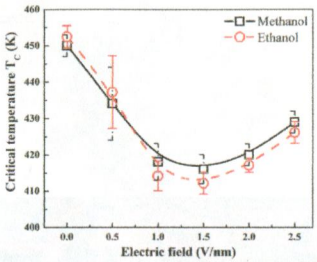


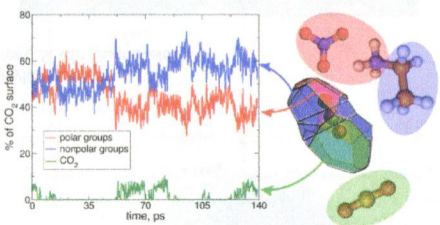
3080 dx.doi.org/10.1021/je500157b

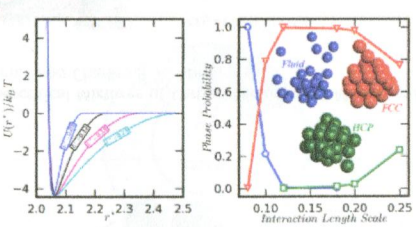
Size-Selective, Noncovalent Dispersion of Carbon Nanotubes by PEGylated Lipids: A Coarse-Grained Molecular Dynamics Study

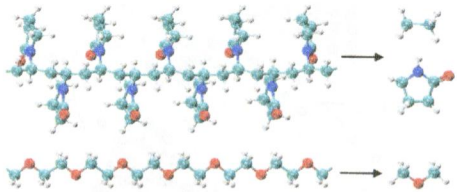
Jukka Määttä, Sampsa Vierros, Paul R. Van Tassel, and Maria Sammalkorpi*

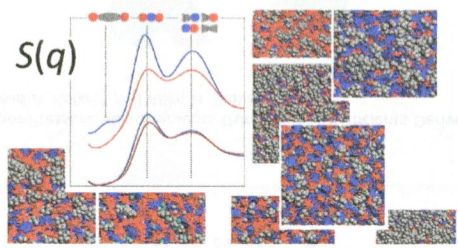


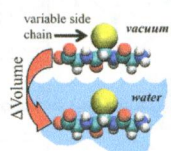


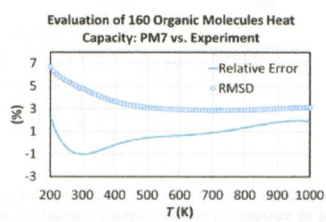










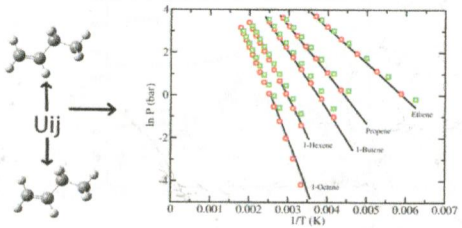


3144 S

dx.doi.org/10.1021/je500202q

Mie Potentials for Phase Equilibria: Application to Alkenes

Jeffrey J. Potoff* and Ganesh Kamath

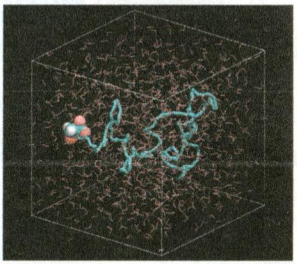


3151 S

dx.doi.org/10.1021/je500211w

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*



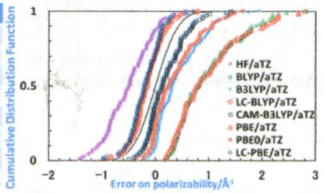
3160 S

dx.doi.org/10.1021/je500224e

Polarizabilities from Long-Range Corrected DFT Calculations

Shintaro Maekawa and Krzysztof Moorthi*

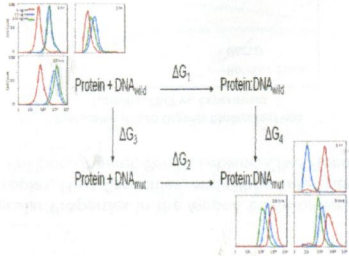
Method	RMSD/Å³
LC-BLYP	0.34
LC-PBE	0.35
CAM-B3LYP	0.42
PBE0	0.59
B3LYP	0.64
HF	0.65
BLYP	1.15
PBE	1.18



3167 dx.doi.org/10.1021/je500225x

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

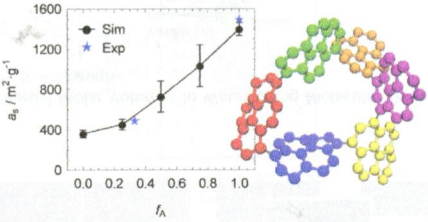
Dan S. Bolintineanu, Katherine Volzing, Victor Vivcharuk, Abdallah Sayyed-Ahmad, Poonam Srivastava, and Yiannis N. Kaznessis*



3177 S dx.doi.org/10.1021/je5002329

Porosity and Ring Formation in Conjugated Microporous Polymers

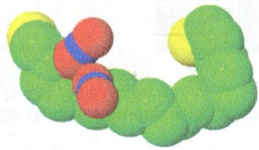
Lauren J. Abbott and Coray M. Colina*



3183 S dx.doi.org/10.1021/je500245f

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

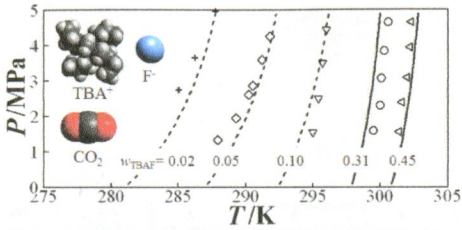
Shu Yang, Andrew J. Schultz, David A. Kofke,* and Allan H. Harvey



3193 dx.doi.org/10.1021/je500243k

Modeling the Dissociation Conditions of Carbon Dioxide + TBAB, TBAC, TBAF, and TBPB Semiclathrate Hydrates

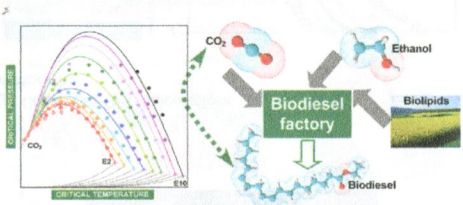
Ayako Fukumoto, Patrice Paricaud,* Didier Dalmazzone, Wassila Bouchafaa, Thi Thu-Suong Ho, and Walter Fürst



3205 dx.doi.org/10.1021/je5002494

Development of a Predictive Equation of State for CO_2 + Ethyl Ester Mixtures Based on Critical Points Measurements

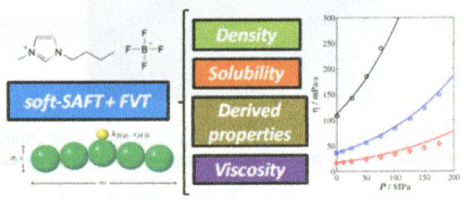
Niramol Juntarachat, Romain Privat,* Lucie Coniglio, and Jean-Noël Jaubert

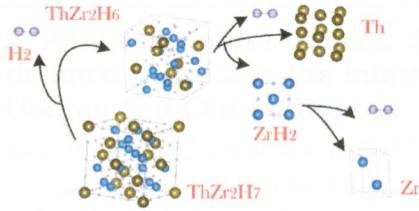


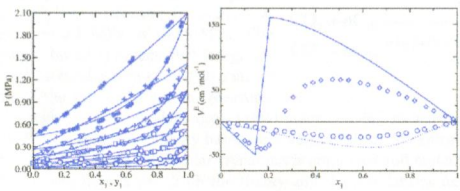
3220 dx.doi.org/10.1021/je5002472

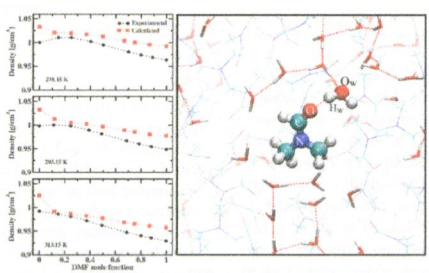
Assessing Ionic Liquids Experimental Data Using Molecular Modeling: $[C_nmim][BF_4]$ Case Study

Felix Llovell* and Lourdes F. Vega





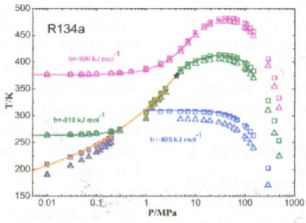




3258 dx.doi.org/10.1021/je500260d

Molecular Simulation for Thermodynamic Properties and Process Modeling of Refrigerants

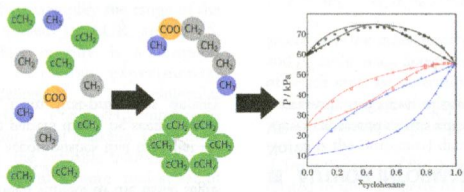
William R. Smith,* Susana Figueroa-Gerstenmaier, and Magda Skvorova



3272 dx.doi.org/10.1021/je500248h

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

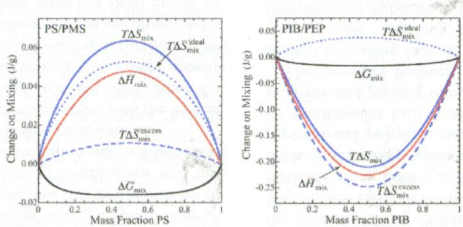
Simon Dufal, Vasileios Papaioannou, Majid Sadeqzadeh, Thomas Pogiatzis, Alexandros Chremos, Claire S. Adjiman, George Jackson, and Amparo Galindo*



3289 dx.doi.org/10.1021/je5002818

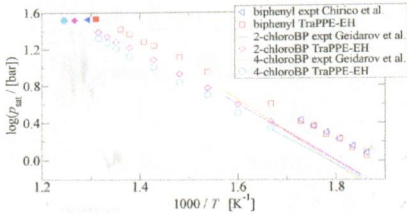
Connecting Theory and Experiment To Understand Miscibility in Polymer and Small Molecule Mixtures

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*



(S) Supporting Information available via online article