

CoMSEF Newsletter

AIChE[®]

October 2010

CoMSEF General Meeting in Salt Lake City

CoMSEF will hold its annual General Meeting on Wednesday November 10th from 6:15-7:15 p.m. during the Fall 2010 AIChE Meeting in Salt Lake City. As in the past, the meeting will be held jointly with Area 1a (Thermodynamics and Transport Properties). All CoMSEF members are encouraged to attend. The winners of the CoMSEF Graduate student awards will be announced and the CoMSEF Early Career Award presented.

CoMSEF Elections

The annual CoMSEF election is currently underway. This year, we will elect a Vice-Chair, two Liaison Directors and a Secretary/Treasurer. Information about the candidates and the duties of each office can be found on the CoMSEF web site at <http://comsef.org/election/2010>. All CoMSEF members can vote in the election and this year we are using Survey Monkey to record your votes. Simply navigate to <http://www.surveymonkey.com/s/PPL6K95> and cast your vote before October 16th.

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David Sholl 2010 CoMSEF Early Career Award Winner



The CoMSEF Executive Committee is pleased to announce that Professor David Sholl of Georgia Tech University has been selected as the recipient of the 2010 CoMSEF Early Career Award. This annual award recognizes outstanding research in computational molecular science and engineering and will be given to David during the CoMSEF annual General Meeting. David is the Michael E. Tennenbaum Family Chair and GRA Eminent Scholar in Energy Sustainability in the School of Chemical & Biomolecular Engineering at Georgia Tech. He has held this position since January 2008 and was previously on the faculty at Carnegie Mellon University for 10 years. He received his undergraduate degree in Physics from the Australian National University and a PhD in Applied Mathematics from the University of Colorado. David's research uses computational materials modeling to accelerate the development of new materials for energy-related applications, including generation and storage of gaseous and liquid fuels and carbon dioxide mitigation. David is a Senior Editor of *Langmuir* and is an Associate Director of the Georgia Tech's Strategic Energy Institute.

David is receiving the CoMSEF Early Career Award for his contributions to the understanding of the thermodynamics and transport properties of hydrogen in solids and of fluids confined in nanoporous materials. CoMSEF Early Career Award recipients must be within 15 years of completion of their highest degree and be current members of CoMSEF.

2010 CoMSEF Graduate Student Awards

The CoMSEF Graduate Student Awards in Computational Molecular Science and Engineering will be awarded for the 6th consecutive year at the annual AIChE Meeting in Salt Lake City. The awards recognize excellence in research by graduate students in the field of computational molecular science and engineering. Two awardees will be selected based on the nomination letters received from each student's advisor and a poster presented at the CoMSEF poster session (session #184) to be held Monday evening from 6 - 8 pm. The winners will be announced at the CoMSEF annual General Meeting (Wednesday November 10th from 6:15-7:15 p.m).

Membership Renewal

It's renewal time. As a CoMSEF member you will receive an electronic copy of our semi-annual newsletter (which highlights CoMSEF activities, opportunities, and recent papers in the literature) and occasional postings about job openings/upcoming conferences. Additionally, as a CoMSEF member you can be nominated (if eligible) for one of the CoMSEF awards.

To renew your membership for another year (including CoMSEF), go to:

<http://www.aiche.org/MemberCenter/Renew.aspx>

CoMSEF will sponsor and co-sponsor 30 technical sessions at the Fall AIChE Meeting

CoMSEF programming at this year's annual meeting will feature a Computational Molecular Science and Engineering Plenary session in which Professors David Sholl and Ed Maginn will present as the recipients of 2009 and 2010 CoMSEF Early Career Awards. The session will also feature contributed talks from CoMSEF members and colleagues chosen by the executive committee for their broad appeal to the CoMSEF community. This session will be an annual feature of CoMSEF programming, so we encourage you to take advantage of this opportunity next year to showcase your work!

Co-Sponsor	Session Name
10,18j	Workshop On National Investment, Policy and Education in Simulation-Based Engineering and Science
10,18j,10e	The Application of Simulation Based Engineering and Science to Industrial Operations and Engineering Management of Enterprise Process Systems: Invited Speakers
10,18j	Innovation and Insight Via High Fidelity Simulation and Large Database Studies of Micro, Macro and Multi-Scale Phenomena: Invited Speakers
1a	In Honor of Stanley Sandler's 70th Birthday I and II
	Plenary Session on Computational Molecular Science and Engineering
	CoMSEF Poster Session
	Recent Advances in Molecular Simulation Methods I and II
15c	Molecular Modeling of Biophysical Processes I – Molecular Binding
15c	Molecular Modeling of Biophysical Processes II – Protein Structure and Dynamics
	First-Principles Simulations of Condensed Phases
8e	Computational Studies of Electronic and Photonic Materials
1a	Industrial Applications of Computational Chemistry and Molecular Simulation I and II
10d, 20	Multiscale Modeling I and II
8a	Modeling and Simulation of Polymers
2e	Molecular Simulation of Adsorption I and II
1a	Computational Studies of Self-Assembly
1a	Computational Studies of Self-Assembly II
1a	Development of Intermolecular Potential Models
20,1g	Computational Catalysis I, II, and III
10d	Numerical Methods for Molecular and Mesoscopic Systems
	The Industrial Fluid Properties Simulation Challenge
10d	Multiscale Modeling for Materials Processing

Research Highlight: Garde group unravels the mysterious hydrophobic interface

By Jeff Errington

Rahul Godawat, Sumanth N. Jamadagni, and Shekhar Garde, "Characterizing hydrophobicity of interfaces by using cavity formation, solute binding, and water correlations", *Proc. Nat. Acad. Sci. USA* **106**, 15119 (2009).

<http://dx.doi.org/10.1073/pnas.0902778106>

Water is commonly found at hydrophobic surfaces in natural systems (e.g. proteins, plant leaves) and numerous emerging technologies (e.g. nanofluidic devices). Despite the importance of such interfaces, our understanding of them is lacking in many ways. In particular, relationships between macroscopic measures of hydrophobicity (e.g. contact angle) and microscopic signatures of hydrophobicity (e.g. depletion layer thickness) are poorly understood. The Garde group recently presented results that bring considerable clarity to this issue. They used molecular dynamics simulation to study water at self-assembled monolayers of alkane-thiol surfactants with a wide range of chemistries that spanned from hydrophobic to hydrophilic in nature. They analyzed the relationships between various microscopic metrics and the contact angle a water droplet forms on the monolayer, a macroscopic property often used to quantify hydrophobicity. They first examined the density of water in the interfacial region, a quantity that is related to the thickness of the so-called depletion layer, wherein water is preferentially excluded from the hydrophobic interface. Given the prevailing view that the thickness of the depletion layer is intimately connected with the hydrophobicity of the surface (increasing depletion layer thickness with increasing hydrophobicity), they expected to find a strong correlation between contact angle and interfacial water density. Instead, they found a surprisingly weak correlation between these two quantities. Moreover, they observed relatively little change in the water density profile upon variation of the surface hydrophobicity. Further analysis revealed a relatively strong correlation between the contact angle and the excess chemical potential for solvation of a hydrophobic solute in the interfacial region. From a physical perspective, the excess chemical potential provides a measure of the probability of cavity formation. Based upon this work, the Garde group established a link between a macroscopic measure of hydrophobicity (the contact angle) and a microscopic aspect of the system (the likelihood of finding nanoscale cavities at the monolayer-water interface). The study highlights the molecular-level insight that one can obtain from the thoughtful application of computer simulation and statistical mechanics.

Research Highlight: Preferential CO Oxidation in Hydrogen: Reactivity of Core-Shell Nanoparticles

By Alberto Striolo

<http://dx.doi.org/10.1021/ja101108w>

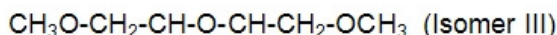
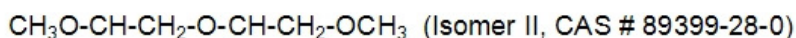
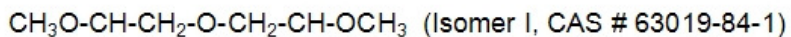
Nilekar et al. [A.U. Nilekar, S. Alayoglu, B. Eichhorn, M. Mavrikakis, *JACS* 132 (2010) 7418-7428], using periodic, self-consistent ab initio DFT calculations, guided the practical synthesis of extremely active catalysts for the PROX reaction at mild conditions. Using the new catalysts, complete CO oxidation was achieved at 30C from a feed containing 1000 ppm CO in hydrogen. This impressive result will lead to significant savings in energy consumption compared to those currently required for the practical application of hydrogen fuel cells.

The novel catalysts are composed by a transition-metal core, covered by a thin (1-2 monolayers at most) Pt shell. The highest catalytic activity has been observed for Ru-Pt core-shell nanoparticles. The catalysts require careful preparation because the core-shell structure just described is not thermodynamically stable. Further, by employing the 'climbing-image nudged elastic band' method, the Authors described in details the elementary reaction steps involved in the preferential CO oxidation in the presence of hydrogen.

This work demonstrates how careful computational-modeling calculations, when coupled with detailed experiments can yield benefits for the entire scientific enterprise.

The Sixth Industrial Fluid Properties Simulation Challenge

By Jonathan Moore



Unlike most organic solvents, glycol ethers and glycol diethers exhibit an "inverse solubility" relationship with water. That is, in the range of normal process conditions they become more compatible as they are cooled and are completely miscible below the lower critical solution temperature (LCST). This behavior is typically rationalized in terms of a temperature-dependent balance between hydrophobic and hydrophilic interactions. This balance of interactions in aqueous solutions is of great scientific and practical importance as a key driving force in phenomena like self-assembly and protein folding. Glycol ethers are used in a wide range of product formulations and industrial processes.

For example, they are used as solvents and co-solvents in both organic- and water-based formulations for applications such as cleaning solutions, paints, coatings, and inks. A variety of other novel applications have been pro-

posed that take advantage of the inverse solubility behavior.

Dipropylene glycol dimethyl ether (DPGDME) is unique among common propylene-oxide-based solvents in that it has no hydroxyl functionality. This means it is relatively inert and can be used in systems that are proton-sensitive (e.g., water-based polyurethane coatings). Although mutual solubility data for liquid-liquid equilibrium (LLE) for a number of water + ethylene glycol ether and water + propylene glycol ether mixtures have been reported in the literature [1], the temperature-dependence of water + dipropylene glycol dimethyl ether mutual solubility has not been reported. Data are available at 298 K for the commercial product PROGLYDE DMM™ where the solubility of DPGDME in water is reported to be 35 wt % and of water in DPGDME to be 4.5 wt % [2]. Proglyde DMM (C₈H₁₈O₃) consists of 3 structural isomers, two of which are the major components that occur in approximately equal amounts). A typical composition of PROGLYDE DMM is 50 % I, 47 % II, and 3 % III. CAS # 111109-77-4 can represent any of the three isomers or mixtures thereof.

Studies of phase equilibria by molecular simulation have become relatively common, employing techniques such as Gibbs Ensemble Monte Carlo [3] and Grand Canonical Monte Carlo with histogram reweighting [4]. Typically, these methods have been employed to study vapor-liquid equilibria in particular and to develop general, transferable force fields (potential energy models) that are reasonably accurate over a wide range of state conditions. Only rarely have these methods been used to predict liquid-liquid equilibria of realistic, moderately complex molecular systems. More commonly, molecular dynamics simulations have been used to study liquid-liquid systems, but those studies have typically focused on the details of structure and interactions at the interface and not on predicting the bulk phase compositions of the coexisting phases. Therefore, assessing the capability of molecular simulation methods and force fields to accurately predict liquid-liquid phase equilibria for practically relevant and moderately complex chemical systems is of interest in establishing more clearly the state-of-the-art capability in this application area.

Challenge

For the PROGLYDE DMM + water system, compute the mutual solubilities in liquid-liquid equilibria at temperatures of 283, 323, 333 and 353 K and atmospheric pressure.

Rules of the Game

- Any theory/modeling/simulation method can be used. In keeping with the focus and goals of the IFPSC, molecular modeling and simulation methods are especially encouraged.
- Any force field (or other model parameterization) previously published in the open literature prior to the announcement of this challenge is acceptable.
- Force fields (or other models) that have not been published previously may not be parameterized for this challenge using mutual solubility data for the water + DPGDME system (except for the published data at 298 K). Force fields (or other models) may be parameterized using any other published physical property data.
- Estimates of the uncertainty for computed mutual solubilities must be included.
- Participants may choose to model PROGLYDE DMM as only one of its constituent isomers or as a mixture of isomers.

Entries are due to contest@ifpsc.org by October 15, 2010, and will be discussed at the IFPSC session at the AIChE Annual Meeting in Salt Lake City:

Tuesday, November 9, 2010: 8:30 AM, 151 A/B Room (Salt Palace Convention Center)

[For more info, see http://fluidproperties.org/6th](http://fluidproperties.org/6th)

References

- [1] S.P. Christensen, F.A. Donate, T.C. Frank, R.J. LaTulip, L.C. Wilson, Mutual Solubility and Lower Critical Solution Temperature for Water + Glycol Ether Systems, *J. Chem. Eng. Data*, 50 (2005) 869-877.
 - [2] Proglyde DMM Product Information
 - [3] A.Z. Panagiotopoulos, Direct determination of phase coexistence properties of fluids by Monte Carlo simulation in a new ensemble, *Mol. Phys.*, 61 (1987) 813-826.
 - [4] A.M. Ferrenberg, R.H. Swendsen, New Monte Carlo technique for studying phase transitions, *Phys. Rev. Lett.*, 61 (1988) 2635-2638.
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Upcoming Conferences of Interest to CoMSEF Members

2011 MRS Spring Meeting

April 25-29, 2011

San Francisco, CA

http://www.mrs.org/s_mrs/sec.asp?CID=21379&DID=246341

ICheaP-10

The tenth International Conference on Chemical & Process Engineering

May 8-11, 2011

Florence, Italy

<http://www.aidic.it/icheap10/>

Midwest Thermodynamics and Statistical Mechanics (MTSM) conference

May 25-27, 2011

Wheaton College, Wheaton IL

5th ESAT meeting

June 24-27, 2011

St. Petersburg, Russia.

19th European Conference on Thermophysical Properties

August 28th - September 1st, 2011

Thessaloniki, Greece

<http://19ectp.cheng.auth.gr/>

Thermodynamics 2011

31st Aug - 2nd Sep 2011

Athens, Greece

<http://www.thermodynamics2011.org/>

8th Liquid Matter Conference

September 6 - 10 2011

Vienna, Austria

<http://lmc2011.univie.ac.at/>