Computational Molecular Science and Engineering Forum
for the combined community of engineers and scientists developing and applying molecularly based theories, modeling, and simulation
http://comsef.org/

CoMSEF Newsletter

AIChE

October 2011

In This Issue

CoMSEF General Meeting in Minneapolis

CoMSEF will hold its annual General Meeting on Wednesday October 19 from 6:15-7:15 p.m. in 101 I (Minneapolis Convention Center) during the Fall 2011 AIChE Meeting. 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 Impact Award presented.

CoMSEF Elections

The annual CoMSEF election is currently underway. This year we will elect two Liaison Directors. Information about the candidates and the duties of each office can be found at http://comsef.org/election/2011. You should have received voting instructions by email. If you didn't receive the email or lost it, send email to admin@comsef.org for help. The deadline for casting your vote is October 19th.

Bernhardt Trout 2011 CoMSEF Impact Award Winner

The CoMSEF Executive Committee is pleased to announce that Professor Bernhardt Trout of the Massachusetts Institute of Technology has been selected as the recipient of the 2011 CoMSEF Impact Award. This annual award recognizes outstanding research in computational molecular science and engineering and will be given to Bernhardt during the CoMSEF General Meeting at the AIChE Annual meeting in Minneapolis. He will also present a talk on his research at the CoMSEF Plenary Session at the AIChE Annual meeting. Bernhardt is the Director of the Novartis-MIT Center for Continuous Manufacturing, Co-Chair of the Singapore-MIT Alliance for Chemical and Pharmaceutical Manufacturing, and a Professor of Chemical Engineering at MIT. He received his Bachelor's and Master's degrees in Chemical Engineering from MIT and a PhD in Chemical Engineering from the University of California, Berkeley. Bernhardt has made important contributions to the development of new computational methods, which he has then applied to the solution of important pragmatic problems; most notable is the impact of his work on the manufacture of pharmaceuticals.

He is receiving the CoMSEF Impact Award "*For the development of generally applicable and widely used molecular computational algorithms and their use to obtain new mechanistic understanding of industrially relevant problems*."

CoMSEF Impact Award recipients must be within 15 years of completion of their highest degree and be current members of CoMSEF.

2011 CoMSEF Graduate Student Awards

The CoMSEF Graduate Student Awards in Computational Molecular Science and Engineering will be awarded for the 7th consecutive year at the annual AIChE Meeting in Minneapolis. 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 students' advisor and a poster presented at the CoMSEF poster session (session #190) to be held Monday evening from 6 - 8 pm in Exhibit Hall B (Minneapolis Convention Center). The winners will be announced at the CoMSEF/Area 1a annual General Meeting (Wednesday, October 19 from 6:15-7:15 pm).

Renew Your Membership and Get a Friend to Join!!

It's renewal time!!! CoMSEF membership is a great way to promote activities and sessions in computational molecular science at the Annual AIChE Meeting. As a CoMSEF member, you will receive an electronic copy of our semi-annual newsletter (which highlights CoMSEF activities, members, opportunities, and recent papers in the literature) and occasional postings about job openings/upcoming conferences. Your membership dues support CoMSEF awards that garner recognition for outstanding graduate students and faculty in computational molecular science and engineering. As a CoMSEF member, you can be nominated (if eligible) for one of the CoMSEF awards. Convince a student or colleague to join! Student membership is FREE!! To renew your CoMSEF membership for another year, go to: http://www.aiche.org/DivisionsForums/Join/index.aspx

FOMMS 2012 – It's Just Around the Corner!!

FOMMS 2012 will be held July 22-26, 2012 at The Resort at The Mountain, nestled in the western highlands of Mt. Hood less than an hour southeast of Portland, Oregon, USA. In addition to outstanding lectures and discussion on a range of topics in molecular modeling and simulation, the conference will include mini-workshops, organized outings, and the FOMMS Medal banquet to honor Professor Keith Gubbins, who is the FOMMS Medal Recipient. For more information or to join the FOMMS email list, go to: http://fomms.org

Important FOMMS dates:

Abstract submission opens:	September 1, 2011
Conference registration begins:	January 4, 2012
Application deadline for fellowships	February 17, 2012
Deadline for submission of poster abstracts:	March 16, 2012
Notification of poster acceptance:	March 30, 2012
Deadline for early registration:	May 31, 2012

Annual Meeting Sessions

CoMSEF will sponsor or co-sponsor 27 sessions at the 2011 AIChE Annual Meeting. Many sessions that have been popular in the past will be continued at this meeting. Several new sessions addressing topical areas will also be introduced. Karl Johnson and Manos Mavrikakis will chair a session titled "**Combining Weak and Strong Forces: Reactive Forcefields and vdW-DFT**". Nonstandard modes of computation will be explored in "**Beyond Standard Hardware: GPUs, Cloud Computing, and Crowdsourcing**", a new session chaired by Peter Cummings, Frank Willmore and Seung Soon Jang. Wei Shi and Robert Enick will chair a session on "**Advances in CO_2 Capture**".

A highlight of the CoMSEF programming will be the **CoMSEF Plenary Session**. Presentations for this session are selected by the CoMSEF executive committee and represent some of the best work from the CoMSEF community. This session will also feature an invited presentation by the CoMSEF Impact Award winner.

A full listing of the CoMSEF sessions is available here: http://aiche.confex.com/aiche/2011/webprogram/21.html

---

Upcoming Conferences of Interest to CoMSEF Members

Conference on Computational Physics
October 30 – November 3, 2011
Gatlinburg, TN
http://ccp2011.ornl.gov/

14th Asia Pacific Confederation of Chemical Engineering Congress 2012
February 21 - 24, 2012
Singapore, Singapore
http://www.rpsonline.com.sg/apcche/
The APCChE 2012 will be held in Singapore on 21 – 24 February 2012. This congress aims to enhance communication among researchers and practitioners from Asian countries working in the area of Chemical Engineering.

APS March Meeting 2012
February 27 - March 2, 2012
Boston, MA
http://www.aps.org/meetings/march/index.cfm

ACS National Meeting and Exposition Spring 2012
March 25-29, 2012
San Diego, CA
http://portal.acs.org/

2012 MRS Spring Meeting
April 9-13, 2012
San Francisco, CA
http://www.mrs.org/spring2012/

Midwest Thermodynamics and Statistical Mechanics (MTSM) conference
May 21-22, 2012
University of Minnesota, Minneapolis, MN
http://www.cems.umn.edu/orgs/MTSM_12

18th Symposium on Thermophysical Properties
June 24-29, 2012
Boulder, CO
http://thermosymposium.boulder.nist.gov/
This triennial symposium is organized by the ASME/AIChE Joint Committee on Thermophysical Properties, provides ample opportunities for oral and poster presentations and informal discussions and takes place on the beautiful CU Boulder campus.

International Conference on Chemical Thermodynamics (ICCT 2012) / CALCON 2012
August 5 - 10, 2012
Búzios, Brazil
http://www.icct2012.org/
The International Conference on Chemical Thermodynamics (ICCT) is held every two years, organized by the International Association for Chemical Thermodynamics (IACT – link – http://iactweb.org) under the auspices of IUPAC.

Research Highlight: Structure Characterization Tools for Porous Materials

By Coray Colina http://dx.doi.org/10.1080/08927022.2011.592832

Lev Sarkisov and Alex Harrison recently published (Molecular Simulation, 2011, forthcoming article) a set of geometric characterization tools applicable to ordered porous materials. The tools include the calculation of surface areas and pore size distributions, as well as analysis of structure connectivity and percolation of the porous space.

Characterization of porous materials is routinely used in the adsorption, membrane and sensor communities, as well as for the design of new materials for desired applications. Sarkisov and Harrison review the “normal practices” of characterizing this type of materials using classical theories such as BET for surface areas or BJH for pore size distributions. They follow with a discussion that acknowledges the challenges of creating structures of disordered porous materials, to then concentrate in the description of the characterization tools for geometric morphology analysis. They show the versatility of the tools through several study cases of MOFs, i.e. crystalline materials. In addition, a design case is included where MOFs with incomplete coordination are created in silico. Their work stresses the importance of accounting for structure connectivity and percolation when performing geometric morphology analyses.

The geometry characterization tools (f90) are available upon request from the authors. Significantly, this set of tools might be applicable (after some modifications) to truly disordered materials such as vycor glasses, activated carbons, porous polymers, and polymers of intrinsic microporosity among others.

The Industrial Fluid Properties Simulation Challenge

By Jonathan Moore

The Industrial Fluid Properties Simulation Challenge (IFPSC, http://fluidproperties.org) is an open competition organized with the goals of driving improvements in the practice of molecular modeling, formalizing methods for the evaluation and validation of simulation results with experimental data, and ensuring relevance of simulation activities to industrial requirements. The Simulation Challenge was initiated by the workshop on "Predicting the Thermophysical Properties of Fluids by Molecular Simulation" and is part of the overall vision of the Industrial Fluid Properties Simulation Collective. The IFPSC session will be held from 12:30 - 3:00 PM on Wednesday October 19 in Conrad B (Hilton Minneapolis). The topic of the 7th IFPSC will be announced and will be accompanied by overview talks highlighting the state-of-the-art in experimental and modeling techniques for adsorption in nanoporous materials. Here is a tentative agenda:

12:30 PM
Introduction and Brief History of the IFPSC
Anne Chaka (NIST)

12:45 PM
The 7th Industrial Fluid Properties Simulation Challenge
Nathan Schultz (3M)

1:15 PM
Modeling Adsorption in Porous Materials
John Brennan and Joshua Moore (Army Research Lab)

2:15 PM
Progress and Challenges in the Physical Adsorption Characterization of Nanoporous Materials
Matthias Thommes (Quantachrome)

The CoMSEF Plenary Session (3:30 PM) will also be located in the Hilton, so make plans to spend your afternoon at that location.

In other news, the journal articles from the 6th IFPSC have recently been published in Fluid Phase Equilibria:

F. H. Case, A. Chaka, J. D. Moore, R. D. Mountain, R. B. Ross, V. K. Shen, and E. A. Stahlberg. "The sixth industrial fluid properties simulation challenge." Fluid Phase Equilib., 310, 1-3 (2011).
http://dx.doi.org/10.1016/j.fluid.2011.07.016

F. A. Donate, K. Hasegawa, and J. D. Moore. "Benchmarks for the sixth industrial fluid properties simulation challenge." Fluid Phase Equilib., 310, 4-6 (2011).
http://dx.doi.org/10.1016/j.fluid.2011.08.014

J. Reinisch, A. Klamt, F. Eckert, and M. Diedenhofen. "Prediction of the temperature dependence of a polyether–water mixture using COSMOtherm." Fluid Phase Equilib., 310, 7-10 (2011).
http://dx.doi.org/10.1016/j.fluid.2011.05.015

P. Bai and J. I. Siepmann. "Gibbs ensemble Monte Carlo simulations for the liquid–liquid phase equilibria of dipropylene glycol dimethyl ether and water: A preliminary report." Fluid Phase Equilib., 310, 11-18 (2011).
http://dx.doi.org/10.1016/j.fluid.2011.06.003

S.-T. Lin, L.-H. Wang, W.-L. Chen, P.-K. Lai, and C.-M. Hsieh. "Prediction of miscibility gaps in water/ether mixtures using COSMO-SAC model." Fluid Phase Equilib., 310, 19-24 (2011).
http://dx.doi.org/10.1016/j.fluid.2011.06.015

T. Köddermann, K. N. Kirschner, J. Vrabec, M. Hülsmann, and D. Reith. "Liquid–liquid equilibria of dipropylene glycol dimethyl ether and water by molecular dynamics." Fluid Phase Equilib., 310, 25-31 (2011).
http://dx.doi.org/10.1016/j.fluid.2011.07.015

L. Zhao, C. Wu, and N. Huang. "Mutual solubilities study for binary mixtures of dipropylene glycol dimethyl ether and water via molecular dynamics simulation and AMOEBA polarizable force field." Fluid Phase Equilib., 310, 32-38 (2011).
http://dx.doi.org/10.1016/j.fluid.2011.06.014