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

2006 Graduate Student Awards in Computational Molecular Science and Engineering

This was the first year for the CoMSEF Graduate Student Awards, which are meant to recognize excellence in research by graduate students in the field of computational molecular science and engineering. We had 13 nominees. The two awardees were selected based on a nomination letter and a poster presentation at the November AIChE meeting in San Francisco. The 2006 awardees are

Megha Surve, University of Texas, Austin

Advisor: Venkat Ganesan

Eric Santiso, North Carolina State University

Advisor: Keith Gubbins

Each winner received a certificate and a cash award at the CoMSEF plenary session.

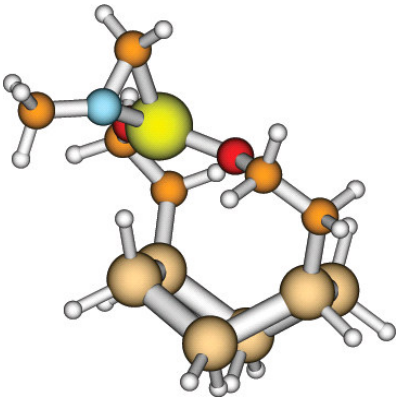
April 2007

In This Issue

Call for Nominations: 2007 CoMSEF Graduate Student Awards

AIChE's Computational Molecular Science and Engineering Forum (CoMSEF) is soliciting nominations for its 2007 graduate student awards recognizing excellence in research by graduate students. The intent of the awards is to reward significant contributions to research in computational molecular science and engineering by students. The award consists of a plaque and an honorarium. Two awards are to be given annually. The 2007 awards will be presented at the special Keith Gubbins session at the AIChE Annual Meeting.

Nominations should consist of a nominating letter from the student's research advisor and the curriculum vitae of the nominee. These should be sent by the advisor via e-mail in pdf format to the CoMSEF Chair, Randy Snurr (snurr@northwestern.edu), by October 1, 2007.



In addition, nominees must present a poster at the CoMSEF Poster session. The deadline for submission of poster abstracts is May 14, 2007.

The nominee must be a graduate student at the time of the poster presentation, and the faculty nominator must be a member of CoMSEF.

Nominations will be selected by a committee composed of CoMSEF officers based on the student's CV, the nomination letter from the advisor, and the quality of the poster presentation.

Please contact Randy Snurr (snurr@northwestern.edu) if you have questions about the award.

Molecular Simulation Modules Proposal Solicitation

CACHE (Computer Aids for Chemical Engineering) has been awarded a new CCLI grant from NSF that is structured to accept proposals from the science/engineering community. The aim is to generate ideas for interactive molecular simulation modules for use in undergraduate instruction. Persons submitting proposals selected for development will receive $5000 as a consulting fee to work with us to develop the module. We can fund 4 of these each year, for three years. Deadline for the first round of proposals is mid-May. More information is available at www.etomica.org (once there, follow the "module solicitation" link).

CoMSEF Sessions for Fall 2007 AIChE Mtg.

CoMSEF will co-sponsor 25 sessions at the Fall 2007 AIChE meeting in Salt Lake City. The call for papers is open through May 14 (link). The preliminary program (list of all sessions) is available online (link). Here is the list of the CoMSEF (Area 21) sessions:

Session Name	Primary Sponsor	Co-Sponsor
CoMSEF Poster Session	21	
First-principles Simulations of Condensed Phases	21	
Keith Gubbins 70th Birthday Celebration	21	1a
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The Fourth International Fluid Properties Simulation Challenge	21	1a
Industrial Applications of Computational Chemistry and Molecular Simulation I	21	1a
Industrial Applications of Computational Chemistry and Molecular Simulation II	21	1a
Recent Advances in Molecular Simulation Methods	21	1a
Multiple Time-scale Modeling in Molecular Simulation	21	10d, 20
Numerical Methods and Simulation of Multiscale Systems I	10d	20, 21
Numerical Methods and Simulation of Multiscale Systems II	20	10d, 21
Numerical methods for molecular and mesoscopic systems	10d	21
Computational Catalysis I	20	1g, 21
Computational Catalysis II	20	1g, 21
20 years of the Gibbs ensemble	1a	21
Development of intermolecular potential models	1a	21
Nucleation and Growth	1a	21
Computational Studies of Self-Assembly	1a	21
Molecular modeling of biophysical processes	15c	21
Molecular modeling of adsorption I	2e	21
Theories of Adsorption	2e	21
Multiscale Modeling & Characterization of Polymers	8a	21
Modeling and simulation of inorganic semiconductor systems	8e	21
Modeling and simulation of organic semiconductor systems	8e	21
Advances in the computation of electronic materials	8e	21

Programming for Spring 2008 AIChE Mtg.

The 2008 Spring AIChE and ACS meetings will be held concurrently in New Orleans. CoMSEF will be taking advantage of this opportunity to program at the Spring meeting by co-sponsor sessions with the Computers in Chemistry Division of the ACS. This should be a great opportunity to have a presence at the Spring meeting and to expand the visibility of CoMSEF within AIChE and ACS. Plans are still in the formative stages, but we have plans for a session in “Computational Evaluation of Rate Constants” and have discussed one or two others in areas such as “Computation of Solid and Fluid Phase Equilibria” or “Modeling of Aqueous Solutions.” Suggestions for topics or volunteers interesting in co-organizing a session with ACS are encouraged to contact Bill Schneider at wschneider@nd.edu or (574) 631-8754.

Molecular simulations and experiments provide new insights into the dynamics of fluids in confined environments

Perla Balbuena

A recent Letter to Nature[1] illustrates the potential of carefully designed combinations of molecular simulations and experiments to elucidate physical phenomena. Dynamic Monte Carlo simulations from Peter Monson's group at the University of Massachusetts not only yield adsorption/desorption isotherms but also clearly explain the dynamic behavior of a confined fluid in the hysteresis region. The pressure dependence of the simulated diffusion data is in excellent qualitative agreement with measurements of adsorption and diffusion in Vycor mesoporous glass, and the analyses of the combined experimental-simulation data conclude with the identification of a novel mechanism of the transient uptake in the hysteresis region.

Reference
(1) Valiullin, R.; Naumov, S.; Galvosas, P.; Karger, J.; Woo, H.-J.; Porcheron, F.; Monson, P. A. Exploration of molecular dynamics during transient sorption of fluids in mesoporous materials, Nature 2006, 443, 965. link

Science Podcasts

Can't get enough science and engineering? Need some listening material for a commute or exercise session? Try a science podcast. Here are links to a few (also available via iTunes):

- Science Friday
- Nature Podcast (Nature Magazine)
- Science Magazine Podcast
- Science Talk (Scientific American)
- 60-Second Science (Scientific American)
- NewScientist.com podcast (New Scientist)
- PopSci Podcasts (Popular Science)
- Technology Review Audiodizer podcasts

New CoMSEF Web Site

The revamped CoMSEF web site is now online at:
http://comsef.org/

It features a variety of content in three categories: 1) publicly-available, 2) for members only, and 3) for the CoMSEF executive committee. For now, the members-only content is limited to the CoMSEF meeting minutes and this newsletter, but we plan to add more content in the near future. We welcome suggestions regarding what types of content would be valuable to CoMSEF members (send suggestions to admin@comsef.org). A username and password are required to access the members-only content, and CoMSEF members should expect to receive theirs in the near future via email.

Special Sessions Honoring Keith Gubbins in Salt Lake City

Two special sessions will be held at the Fall 2007 AIChE meeting in honor of Keith Gubbins' 70th birthday and in recognition of his contributions to chemical engineering.

2006-2008 CoMSEF Executive Committee

In 2006 several CoMSEF Executive Committee roles (including vice-chair and program chair, secretary-treasurer, and 2 liaison directors) were filled by election and others (vice chairs for communications and membership) were filled by appointment of the chair. The Executive Committee is:

Chair	Randy Snurr
Vice-Chair and Program Chair	Clare McCabe
Secretary-Treasurer	Joe Golab
Vice Chair for Communications	Jonathan Moore
Vice Chair for Membership	Dave Kofke
Program Chair for Spring 2008	Bill Schneider
Liaison Director (2004-2006)*	Ken Cox
Liaison Director (2004-2006)*	Sanat Monhanty
Liaison Director (2006-2008)	Perla Balbuena
Liaison Director (2006-2008)	Roland Faller
Past Chair	Paulette Clancy

* Note that the 2004-2006 liaison directors will serve an extra year (2006-2007)

AIChE Centennial Celebration

AIChE will be celebrating its centennial in 2008. The Centennial will give AIChE the opportunity to highlight the contributions of chemical engineers to society's well being and standard of living, recognize the Institute's accomplishments, and envision an even brighter future for chemical engineering. (link)

If you have any ideas could celebrate the AIChE's centennial, please forward them to the CoMSEF executive committee (admin@comsef.org).

News Briefs

- **Seed Magazine: Science In Silico**: "*Computer simulations and visualizations are performing the thought experiments of the 21st century and pushing the limits of human vision and imagination.*" (link to more)
- **Science and Engineering Visualization Challenge**: (link to more)
- **Computational high-throughput screening of electrocatalytic materials for hydrogen evolution**: "*In this contribution, we present a density functional theory-based, high-throughput screening scheme that successfully uses these strategies to identify a new electrocatalyst for the hydrogen evolution reaction (HER).*" Nature Materials (link to more)
- **Horst Simon Steps Down As NERSC Director**: *"Horst Simon, who has been director of DOE's National Energy Research Scientific Computing Center (NERSC) since early 1996, announced last month that he was stepping down in order to focus his energy on the two other positions he holds at Lawrence Berkeley National Laboratory...Simon took some time to talk about his decision and how he sees his future. "* (link to more)
- **Cutting-Edge Projects Awarded Computing Time On Blue Gene/L**: "*Nine computing projects ranging from predicting protein structure to simulating the formation of foams have been awarded large amounts of time on IBM Blue Gene/L computer systems at the U. S. Department of Energy's Argonne National Laboratory and IBM's T.J. Watson Research Center in Yorktown Heights, N.Y. The computer time is available to researchers through the Department of Energy's INCITE program – Innovative and Novel Computational Impact on Theory and Experiment.*" (link to more)
- **17th Machine Evaluation Workshop at Daresbury**: "*On December 4th through 6th, 2006, about 250 people (around the same as last year) attended the 17th machine evaluation workshop at CCLRC Daresbury Laboratories, UK. This excellent workshop, in its seventeenth year, is a leading UK national event dedicated to distributed, high performance scientific computing.*" (link to more)
- **Atomistic Simulator Helps Students Visualize Big Problems**: "*...students can learn to apply sophisticated atomistic modeling techniques to traditional materials research in just a few classes, an advance that could dramatically change the way civil engineers learn to model the mechanical properties of materials and provide enormous benefit to industry.*" (link to more)
- **Pressure Dependence of the Radial Breathing Mode of Carbon Nanotubes: The Effect of Fluid Adsorption**: "*Using analytical methods as well as molecular simulation, we observe a low frequency breathing mode for the adsorbed fluid...*" Phys. Rev. Lett. (link to more)
- **Multiscale Modeling of Liquids with Molecular Specificity**: "*The separation between molecular and mesoscopic length and time scales poses a severe limit to molecular simulations of mesoscale phenomena. We describe a hybrid multiscale computational technique which addresses this problem by keeping the full molecular nature of the system where it is of interest and coarse graining it elsewhere.*" Phys. Rev. Lett. (link to more)
- **Freezing of Fluids Confined in a Disordered Nanoporous Structure**: "*Freezing of a simple fluid in a disordered nanoporous carbon is studied using molecular simulations.*" Phys. Rev. Lett. (link to more)