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

May 2008

In This Issue

CoMSEF Elections Fall 2008

This Fall we will hold elections for Vice-Chair, Secretary-Treasurer, and two Liaison Directors. In accordance with our by-laws, a slate of candidates will be drafted by the current officers and then additional candidates solicited from the CoMSEF membership. Members interested in running for an officer position or getting more involved in CoMSEF in some other way should contact Randy Snurr (snurr@northwestern.edu) or Clare McCabe (c.mccabe@vanderbilt.edu).

CoMSEF Programming at the Spring 2008 AIChE Meeting

William F. Schneider

The Spring 2008 ACS and AIChE meetings were concurrent and co-located in New Orleans this year, and to take advantage of the opportunity to do joint programming, CoMSEF co-sponsored several highly successful symposia with the ACS Computers in Chemistry Division. Symposia included "Computational Evaluation of Rate Constants," organized by Herbert da Costa and Thanh Truong, "Computational Phase Equilibria,"organized by Ilja Siepmann and Karl Johnson, and "Computational Catalysis," organized by Suljo Linic and Andrew Rappe. Thanks go to all the organizers for putting together these top-notch scientific programs, which occupied nine half-day sessions and attracted more than 50 oral contributions. These sessions were particularly important for raising the visibility of CoMSEF both with Spring AIChE attendees and with the ACS community and to encouragement for doing joint programming with ACS again when the opportunity arises.

2007 Graduate Student Awards in Computational Molecular Science and Engineering

Congratulations to the 2007 CoMSEF Graduate Student Award winners:

- Chethan Acharya, University of Alabama
  Advisor: C. Heath Turner
- Harish Vashisth, Drexel University
  Advisor: Cameron Abrams

Each winner received a certificate and a cash award. These awards recognize excellence in research by graduate students in the field of computational molecular science and engineering. The awardees were selected based on a nomination letter, CV, and a poster presentation at the November AIChE Meeting in Salt Lake City.

Free COMSEF Membership for Students

AIChE's ScaleUp program provides complimentary AIChE student membership for interested U.S. undergraduate students. This is a new AIChE initiative and is designed to facilitate the relationship between undergraduate students, industry and AIChE. ScaleUp is made possible by sponsorship from BP, Rohm & Haas, DuPont, Praxair, Merck, Dow and UOP. As part of this program COMSEF is pleased to announce that it will offer free membership to undergraduate students, so please enourage any undergraduates that you may have working with you to get involved!

More information for students on the ScaleUp program can be found on AIChE's web site at:
http://www.aiche.org/Students/Join/index.aspx

Information for potential sponsors can be found at:
http://www.aiche.org/About/Foundation/CorporateCampaign/ScaleUp.aspx

Research Highlight: New approach to investigate molecular diffusion at an interface

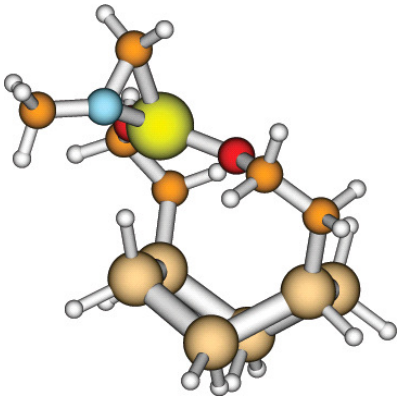
Perla Balbuena

A recent article by D. Duque, P. Tarazona, and E. Chacón, J. Chem. Phys. 128, 134704, (2008) introduces the intrinsic sampling method to investigate the structure and dynamics of molecules at the liquid-vapor interface using molecular dynamics simulations. The analysis and conclusions are very relevant to a variety of complex interfaces existent in many technological applications such as those involving confined water or aqueous solutions, liquid-solid interfaces, and membranes. One of the interesting conclusions of this article is that the typical time required for a molecule to travel a distance of the order of one molecular diameter is comparable to the residence time of the molecules entering or leaving the interfacial region, therefore the presence of that microscopic mass transfer can not be ignored when analyzing diffusion coefficients at the interface.

Call for Nominations: 2008 CoMSEF Graduate Student Awards

AIChE's Computational Molecular Science and Engineering Forum (CoMSEF) is soliciting nominations for its 2008 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 given annually. The 2008 awards will be presented at the AIChE Annual Meeting in Philadelphia.

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, 2008**. Note that the nomination letter and CV are required and are important parts of the nomination; this is not just a poster competition.



In addition, nominees must present a poster at the CoMSEF Poster session. The deadline for submission of poster abstracts is **May 11, 2008**.

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.

CoMSEF will sponsor and co-sponsor 20 technical sessions at the Fall AIChE Meeting

Session #	Session Name
21000	Overview of An International Assessment of Research and Development in Simulation-Based Engineering and Science
21001	Poster Session: Computational Molecular Science and Engineering Forum
21002	First-Principles Simulations
21003	Integrated Multiscale Molecular Simulation
21004	Symposium Honoring H. Ted Davis I
21005	Symposium Honoring H. Ted Davis II
21006	The Fifth Industrial Fluid Properties Simulation Challenge
21007	Industrial Applications of Computational Chemistry and Molecular Simulation I
21008	Industrial Applications of Computational Chemistry and Molecular Simulation II
21009	Recent Advances in Molecular Simulation Methods
01A09	Computational Studies of Self-Assembly
02E04	Molecular Simulation of Adsorption I
02E05	Molecular Simulation of Adsorption II
08A03	Structure and Properties of Polymers III: Networks and Gels
10D10	Numerical Methods for Molecular and Mesoscopic Systems
15C13	Molecular Modeling of Biophysical Processes I
15C20	Molecular Modeling of Biophysical Processes II
20013	Computational Catalysis I
20014	Computational Catalysis II
20030	Multiscale Modeling I
20031	Multiscale Modeling II
TH024	The Evolution of Molecular Modeling into a Chemical Engineering Tool

More details on each of the sessions listed below, and the full meeting program, can be found at http://aiche.confex.com/aiche/2008/preliminaryprogram/index.html.

Participants should note that there are many activities taking place at the fall meeting to celebrate AIChE's centennial, which will likely be concentrated on Sunday - Tuesday (both day and evening) and could result in the scheduling of business meetings and receptions at alternate times. The call for papers is open through May 11th 2008.