

CoMSEF Newsletter

AIChE[®]

April 2011

New Officers

During the fall of 2010, we elected a Vice-Chair and two new Liaison Directors. Congratulations to the newly-elected officers and thanks to all who participated!

Vice-Chair (2010-2012)

- **David Sholl** (Georgia Tech.)

Liaison Directors (2010-2012):

- **Arthi Jayaraman** (University of Colorado Boulder)
- **Monica Lamm** (Iowa State University)

Thanks also to the two out-going Liaison Directors, Alberto Striolo and Jeff Errington, as well as to Past-Chair Randy Snurr, for their participation! A complete listing of the CoMSEF Executive Committee is available on the web:

<http://comsef.org/executivecommittee>

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Become a CoMSEF Officer!

In 2011 we will be holding elections for two Liaison Director positions. Liaison Directors serve two-year terms, and their responsibilities include:

- Facilitate programming with other organizations by identifying opportunities for co-sponsorship
- Communicate and advocate CoMSEF activities with other organizations.
- As members of the Executive Committee, aid the other officers in developing and carrying out CoMSEF activities and preparing the CoMSEF newsletter.

If you would like to get involved in CoMSEF and run for one of these elected positions, please contact any of the CoMSEF officers who can discuss the details with you. You can also find out more information on the CoMSEF web page under the forum bylaws (<http://comsef.org/bylaws>). We are always looking for new people to get involved with new ideas to keep CoMSEF active and relevant so don't be shy and volunteer!

2010 Graduate Student Awards in Computational Molecular Science and Engineering

Congratulations to the 2010 CoMSEF Graduate Student Award winners:

Sumeet C. Pandey (University of Massachusetts Amherst)
Advisor: Dimitrios Maroudas

Diwakar Shulka (Massachusetts Institute of Technology)
Advisor: Bernhardt Trout

Our winners are pictured here with the CoMSEF officers that presented the awards: Left to Right: Dave Kofke (Chair of Grad Student Award Committee); Clare McCabe (CoMSEF Past Chair); Sumeet Pandey; Diwakar Shulka. Each winner received a certificate and cash award.

The awards recognize excellence in research by graduate students in the field of computational molecular science and engineering. The awardees were selected on the basis on a nomination letter from the advisor (who must be a member of CoMSEF), their CV, and their poster presentation at the Fall AIChE Meeting in Salt Lake City.



2011 Impact Award in Computational Molecular Science and Engineering

CoMSEF is soliciting nominations for the 2011 CoMSEF Impact Award, which recognizes outstanding research in computational molecular science and engineering by a member of CoMSEF. Previous award winners include Ed Maginn (2009) and David Sholl (2010).

Nominees for the 2011 award may hold positions in academia, industry, or a national laboratory, and must be within 15 years of completion of their highest degree. Candidates earning PhD degrees from 1996 onwards are award eligible. Nominees must be current members of CoMSEF.

A nomination package consisting of the nominee's CV, a nomination letter and two supporting letters of recommendation should be sent as a single file in pdf format to the CoMSEF Chair, Kristen Fichthorn (fichthorn@psu.edu). The nomination should provide a clear statement as to the impact of the nominee's work on the field and an award citation of 25 words or less, beginning with the word 'For'. Self-nominations are discouraged. The deadline for receipt of nominations will be **May 1st** for the 2011 award with the recipient being announced prior to the Fall AIChE meeting.



David Sholl accepts the 2010 award from Clare McCabe

Please note that renomination of candidates is encouraged. It is recommended but not required that the contents of the nomination package be updated each year; while supporting letters may be re-used, the nomination form must have current dates.

The award recipient will be chosen based on the overall strength of the research accomplishments of the candidates by an ad hoc selection committee consisting of the current CoMSEF chair, the CoMSEF vice-chair and two representatives drawn from related organizations (e.g., area 1a committee, CACHE trustees). Please contact Kristen Fichthorn (fichthorn@psu.edu) with any questions regarding eligibility or the nomination process.

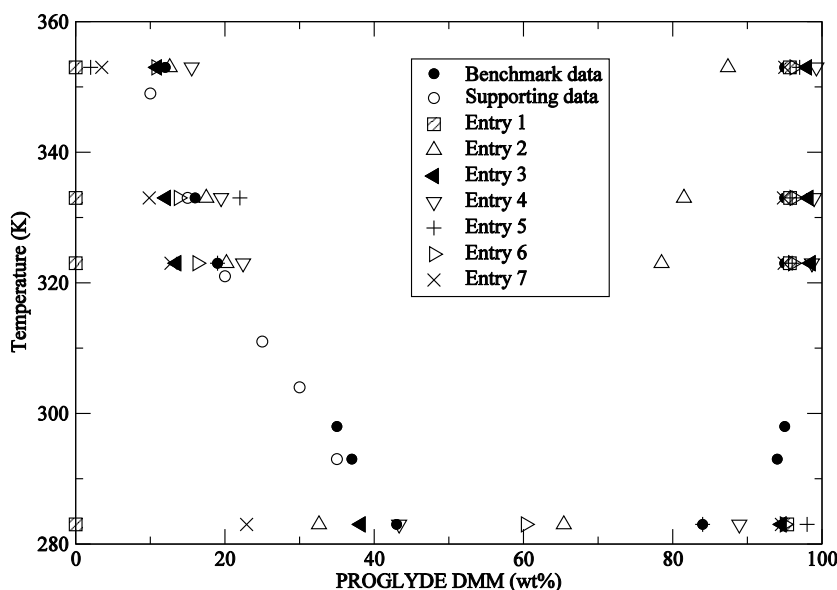
Results of the Sixth Industrial Fluid Properties Simulation Challenge

The results of the Sixth Industrial Fluid Properties Simulation Challenge were announced at a special session at the AIChE Annual Meeting in Salt Lake City in November 2010. Entrants were challenged to predict the mutual solubility in liquid-liquid equilibria of water and a glycol ether (PROGLYDE DMM™) as a function of temperature. Unlike most organic solvents, glycol ethers and glycol diethers exhibit an "inverse solubility" relationship with water. They 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 proposed that take advantage of the inverse solubility behavior.

Seven entries were received, and they were judged based on comparison to experimental data provided by The Dow Chemical Company.

J. Reinisch, A. Klamt, F. Eckert and M. Diederhosen (COSMOlogic) were named Champions. P. Bai and J.I. Siepmann (U. Minnesota) were named Runners-Up. S.-T. Lin, L.-H. Wang, W.-L. Chen, P.-K. Lai, and C.-M. Hsieh (National Taiwan University) were named Honorable Mention.

The other four entries were honored for participating: T. Koddermann, K. N. Kirschner, J. Vrabec, M. Huls-mann, D. Reith (SCAI; U. Paderborn); A. Vahid, F. S. Emami, E. Moharrer, J. R. Elliott (U. Akron); T. Cheng, F. Li, J. Dai, and H. Sun (Shanghai Jiao Tong University); and L. Zhao, C. Wub, and N. Huang (National Institute of Biological Sciences, Beijing, China; Washington University).

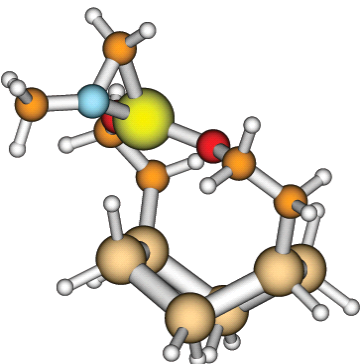


Thanks to all who participated in planning and judging the challenge and to the entrants! A set of journal articles summarizing the 6th Challenge will be published in an upcoming issue of Fluid Phase Equilibria. Please consider participating when the next challenge is announced! For more information about the challenge see: <http://fluidproperties.org/>

Call for Nominations: 2011 CoMSEF Graduate Student Awards

CoMSEF is soliciting nominations for the 2011 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 certificate and an honorarium. Two awards are to be given annually. The 2011 awards will be presented at the Annual Meeting in Minneapolis.

Nominations should consist of a nominating letter from the student's research advisor and the CV of the nominee. We encourage advisors to note that these documents form an important part of the decision process; this is not just a poster competition. **The nominee must be a graduate student at the time of the poster presentation and the faculty nominator must be a member of CoMSEF.** The nomination should be sent as a single pdf file via e-mail from the advisor to the CoMSEF Chair, Kristen Fichthorn (fichthorn@psu.edu), by [October 1, 2011](#).



In addition, nominees must submit an abstract to the CoMSEF Poster session. The deadline for submission of poster abstracts is [May 2, 2011](#).

The winners will be selected by a committee composed of CoMSEF officers based on the student's CV, the nomination letter from the advisor (who must be a member of CoMSEF), and the quality of the poster presentation.

Please contact Kristen Fichthorn (fichthorn@psu.edu) if you have questions about the award.

RESEARCH HIGHLIGHT: Development of coarse-grained model of DNA with explicit coarse-grained water and counterions

By: Arthi Jayaraman

DeMille RC, Cheatham TE, Molinero V J. Phys. Chem. B, 2011, 115 (1), pp 132–142

DOI: <http://dx.doi.org/10.1021/jp107028n>

Molecular simulations have played a critical role in understanding complex biological phenomena, especially those involving macromolecules such as proteins and DNA. One of the challenges faced by computational scientists in this area is maintaining all the chemically- and biologically-relevant details of the system while also reaching the length- and time-scales that are computationally feasible. In this regard, much effort has gone into the development of coarse-grained (CG) models for DNA and proteins with improved CG representation of solvation and electrostatics, in order to accurately mimic the structure and thermodynamics of the biomacromolecule in its physiological environment. In this direction, recent work by Demille et al. (J Phys. Chem. B, 115, 2011, pp132-142) involving development and validation of a CG model of DNA with explicit CG water and ions is an effort worth highlighting. They have combined the mW-ion model developed by DeMille and Molinero (J Chem. Phys. 2009, 131 034107) and the CG DNA model and force field (3SPN) developed by de Pablo and co-workers (J Chem. Phys. 2007, 126, 084901), the latter being able to reproduce several key features of DNA, to produce a coarse-grained model of DNA with an explicit coarse-grained representation of water and ions. They have validated this integrated mW/3SPN-DNA model by reproducing the solvation structure seen in purely atomistic simulations and the relative residence times of water and ions on the DNA molecules. This work by DeMille et al. overcomes limitations of i) atomistic simulations involving explicit solvation, which while becoming more feasible with recent developments in hardware and software remain intractable for long time and length scales, and ii) past CG implementations involving implicit solvation of DNA that do not effectively capture explicit solvent-mediated interactions. This explicitly solvated mW/3SPN-DNA model could be useful in many studies involving DNA (e.g. plasmid supercoiling, gene delivery) or could be extended to other biological systems where solvation and hydrophilic/hydrophobic interactions play a key role in the microscopic behavior of the biomacromolecules.

Free CoMSEF Membership for Students

CoMSEF is pleased to announce that it will offer free membership to undergraduate students as part of AIChE's ScaleUp program. ScaleUp is an AIChE initiative that provides complimentary AIChE student membership to interested U.S. undergraduate students and is designed to facilitate the relationship between undergraduate students, industry and AIChE. ScaleUp is made possible by sponsorship from BP, Air Products, Dow, DuPont, Praxair, Merck, Rohm & Haas, and UOP. Please encourage any undergraduates that you advise or have working with you to get involved!

It's Not Too Early to Plan for FOMMS 2012!

FOMMS 2012 will be held **July 22-26, 2012** at The Resort at Mount Hood in Oregon, about 45 minutes east of Portland. This will be the fifth triennial FOMMS conference. We typically have 100 - 150 international participants, in an interdisciplinary mix that includes chemical engineers, chemists, physicists, and materials scientists from academia (including students and postdocs), government laboratories, and industry. The FOMMS meeting is a Gordon-style conference, with 40-minute invited talks (plus ample discussion time) in the mornings and afternoons, as well as poster sessions for contributed papers. We also hold evening hands-on workshops/discussion sessions on research and educational topics. A good amount of free time is built into the schedule for scientific discussions and activities are planned that take advantage of the beautiful surroundings, including hiking, kayaking and historical tours. More information on FOMMS 2012 and previous conference programs can be found at the conference website at <http://www.fomms.org>.

The programming committee for FOMMS 2012 has assembled a fantastic slate of invited speakers and the conference is certain to be stimulating. In addition, **Professor Keith Gubbins** is the winner of the 2012 FOMMS Medal and will present an award lecture. We hope to see you there!!!

Annual Meeting Sessions

CoMSEF will sponsor or co-sponsor 27 sessions at the 2011 AIChE Annual Meeting (October 16-21, 2011 in Minneapolis, MN). Abstracts for presentations at the meeting will be accepted via AIChE's online system until May 2, 2011. 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 CO₂ Capture**".

A highlight of the CoMSEF programming will be the **CoMSEF Plenary Session**. Presentations for this session are selected by the CoMSEF executive committee, so submitting your best work to this session is a great opportunity to highlight your accomplishments. This session will also feature an invited presentation by the CoMSEF Impact Award winner.

Upcoming Conferences

Thermodynamics 2011

September 1 - 3, 2011

Athens, Greece

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

The "Thermodynamics 2011" conference is the 22nd meeting in a series of thermodynamics conferences founded in the 1960s by John Rowlinson and Max McGlashan.

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.

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.