

CoMSEF Newsletter

AIChE[®]

May 2009

CoMSEF Elections Update

During the fall of 2008, we elected a Vice Chair, a Secretary/Treasurer, and 2 Liaison Directors. Congratulations to the newly-elected officers and thanks to all who participated!

- Vice-Chair and Program Chair: **Kristen Fichthorn** (Penn State)
- Secretary-Treasurer: **Joe Golab** (Ineos)
- Liaison Directors (2008-2010) **Alberto Striolo** (U. Oklahoma) and **Jeffrey Errington** (SUNY Buffalo)

This Fall we will hold elections for 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 Clare McCabe (c.mccabe@vanderbilt.edu).

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Announcing the CoMSEF Early Career Award

We are pleased to announce a new annual CoMSEF award to recognize outstanding research in computational molecular science and engineering. The award will be given for the first time in 2009 and will consist of a plaque and honorarium.

Nominees may hold positions in academia, industry, or a national laboratory, and must be in the early stages of their professional careers, defined as being within 15 years of completion of the highest degree. For the 2009 award, candidates earning PhD degrees from 1994 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, Clare McCabe (c.mccabe@vanderbilt.edu). Self-nominations are discouraged. The deadline for receipt of nominations will be July 1st for the 2009 award with the recipient being announced prior to the Fall AIChE meeting.

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 Clare McCabe (c.mccabe@vanderbilt.edu) with any additional questions about this new award.

2008 Graduate Student Awards in Computational Molecular Science and Engineering

Congratulations to the 2008 CoMSEF Graduate Student Award winners:

- **Rachel Getman**, University of Notre Dame (CoMSEF member Advisor Bill Schneider)
<http://www.nd.edu/~rgetman/>
- **Jeremy Purvis**, University of Pennsylvania (CoMSEF member Advisor Scott Diamond)
<http://www.seas.upenn.edu/~diamond/StaffPages/Purvis.html>

Each winner received a certificate and a \$500 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, the nominees CV, and their poster presentation at the Fall AIChE Meeting in Philadelphia.

Free CoMSEF Membership for Students

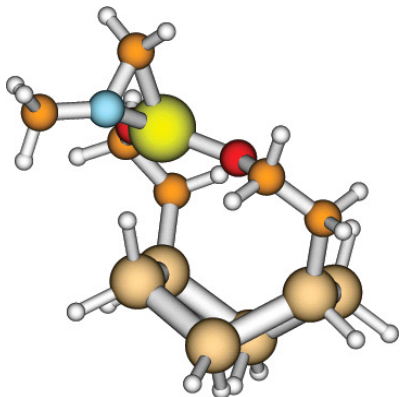
CoMSEF is pleased to announce that it will offer free membership to undergraduate students as part of AIChE's ScaleUp program. ScaleUp is an AIChE initiative that provides complimentary AIChE student membership to interested U.S. undergraduate students and is designed to facilitate the relationship between 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!

CoMSEF will sponsor and co-sponsor 17 technical sessions at the Fall AIChE Meeting

New Proposals to Present may be submitted until: Monday, May 11, 2009 at 11:59pm (EST)

Co-Sponsor	Session
	Chemistry and Kinetics Integrated CFD Modeling Chairs: Joseph T. Golab and Dale Snider
	First-Principles Simulations of Condensed Phases Chairs: Lev D. Gelb and Xiongce Zhao
	Industrial Applications of Computational Chemistry and Molecular Simulation I Chairs: Jonathan Moore and Joseph T. Golab
	Industrial Applications of Computational Chemistry and Molecular Simulation II Chairs: Martin Sanborn and Phillip R. Westmoreland
	Multi-Scale Modelling I Chairs: Abhijit Chatterjee and Talid R. Sinno
	Multi-Scale Modelling II Chairs: Yiannis N. Kaznessis and Kristen A. Fichthorn
	Opportunities for Chemical Engineering in Petascale Computing [Invited Talks Only] Chairs: Sharon C. Glotzer and Peter T. Cummings
	Poster Session: Computational Molecular Science and Engineering Forum Chairs: Kristen A. Fichthorn and Clare McCabe
	Recent Advances in Molecular Simulation Methods Chairs: Michael R. Shirts and Heath Turner
Area 1A	Thermodynamics of Energy Systems Chairs: Hugh Docherty and Maaïke C. Kroon
Area 1A	Computational Studies of Self-Assembly Chairs: Alberto Striolo and Hank Ashbaugh
Area 1A	Development of Intermolecular Potential Models Chairs: Jeffrey Potoff and Ganesh Kamath
Area 8A	Multiscale Modeling and Characterization of Polymers Chairs: Manolis Doxastakis and Ahmed E. Ismail
Area 15C	Molecular Modeling of Biophysical Processes I Chairs: Yiannis Kaznessis and Elaine R. Chan
Area 15C	Molecular Modeling of Biophysical Processes II Chairs: Jhih-Wei Chu and Ravi Radhakrishnan
Area 20	Computational Catalysis I Chairs: John R. Kitchin and Randall J. Meyer
Area 20	Computational Catalysis II Chairs: William F. Schneider and Andreas Heyden
Area 2E	Molecular Simulation of Adsorption I: Chairs: Alexander V. Neimark and Francisco R. Hung
Area 2E	Molecular Simulation of Adsorption II: Chairs: Peter A. Monson and Alberto Striolo

Call for Nominations: 2009 CoMSEF Graduate Student Awards



AIChE's Computational Molecular Science and Engineering Forum (CoMSEF) is soliciting nominations for its 2009 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 2009 awards will be presented at the Annual Meeting in Nashville.

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 nomination should be sent by the advisor via e-mail in pdf format to the CoMSEF Chair, Clare McCabe (c.mccabe@vanderbilt.edu), by October 1, 2009.

In addition, nominees must present a poster at the CoMSEF Poster session. The deadline for submission of poster abstracts is May 11, 2009.

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.

Request for Feedback

The officers of CoMSEF solicit your feedback about the forum and ways it could serve you better. If you have any ideas or suggestions about CoMSEF, its activities, or the content of future newsletters, please send them to admin@comsef.org

CoMSEF Officers

Chair
Clare McCabe (Vanderbilt)

Vice-Chair and Program Chair
Kristen Fichthorn (Penn State)

Secretary-Treasurer
Joe Golab (Ineos)

Vice Chair for Communications
Jonathan Moore (Dow Chemical)

Vice Chair for Membership
Dave Kofke (SUNY Buffalo)

Liaison Director (2008-2010)
Alberto Striolo (Oklahoma)

Liaison Director (2008-2010)
Jeffrey Errington (SUNY Buffalo)

Liaison Director (2007-2009)
Ed Maginn (Notre Dame)

Liaison Director (2007-2009)
Brian Peterson (Air Products)

Past Chair
Randall Snurr (Northwestern)