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

New Officers

During the fall of 2009, we elected 2 new Liaison Directors. Congratulations to the newly-elected officers and thanks to all who participated!

Liaison Directors (2009-2011):

- **Coray Colina** (Penn State U.)
- **J. Ilja Siepmann** (U. Minnesota)

Thanks also to the 2 out-going Liaison Directors, Ed Maginn and Brian Peterson, for their participation! A complete listing of the CoMSEF Executive Committee is available on the web: http://comsef.org/executivecommittee

In This Issue

New CoMSEF Plenary Session

At the 2010 annual AIChE meeting there will be a Computational Molecular Science and Engineering Forum Plenary Session. This session will be a regular addition to CoMSEF programming at the annual meeting and, as a plenary session, will be held without concurrent CoMSEF sessions. The session will feature an invited presentation by the CoMSEF Early Career Award winner, as well as contributed talks from CoMSEF members and colleagues. As such, the papers presented in this session are expected to be of broad appeal to the CoMSEF community and of exceptional quality. Please consider sending an abstract to this session to take advantage of the opportunity to showcase your work to the CoMSEF and AIChE community. Oral presentations from the contributed abstracts will be chosen by ballot of the CoMSEF executive committee.

Become a CoMSEF Officer!

In 2010 we will be holding elections for several officer positions. These will be:

- Vice-Chair, which is a two-year position on the executive committee that leads to the position of Chair (a two-year term) and past Chair (also a two-year term). The Vice-Chair is in charge of programming within AIChE.
- Two Liaison Directors, which are two-year positions.
- Secretary-Treasurer, which is a two-year position.

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 of these positions 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!

2009 Graduate Student Awards in Computational Molecular Science and Engineering

Congratulations to the 2009 CoMSEF Graduate Student Award winners who were Gloria A. E. Oxford from Northwestern University and Dimitrios Argyris from the University of Oklahoma. Our winners are pictured here with their advisors, CoMSEF members, Randy Snurr and Alberto Striolo. 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, the nominees CV, and their poster presentation at the Fall AIChE Meeting in Nashville.

2010 CoMSEF Early Career Award

CoMSEF is also soliciting nominations for the 2010 CoMSEF Early Career Award, which recognizes outstanding research in computational molecular science and engineering by a member of CoMSEF. The award was given for the first time in 2009 to Ed Maginn of the University of Notre Dame, shown below receiving his award from current CoMSEF Chair Clare McCabe. Ed received the Early Career Award *for his development of molecular simulation algorithms to study fundamental thermodynamics and transport behavior and his specific contributions to the understanding of nanoporous materials and ionic liquids.*

Nominees for the 2010 award 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. Candidates earning PhD degrees from 1995 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 is May 1st for the 2010 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 questions regarding eligibility or the nomination process. See also: http://www.aiche.org/About/Awards/Divisions/CoMSEFEarlyCareer.aspx

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Upcoming Conferences

Water & Aqueous Solutions Gordon Conference
August 8-13, 2010
http://www.grc.org/programs.aspx?year=2010&program=water

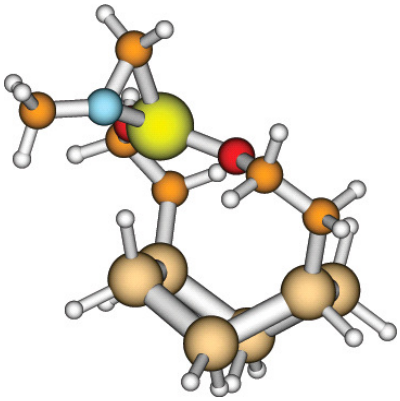
ACS Fall Meeting
August 22-26, 2010
http://portal.acs.org/portal/PublicWebSite/meetings/fall2010/index.htm

AIChE Annual Meeting
November 7-12, 2010
http://www.aiche.org/Conferences/AnnualMeeting/index.aspx

Call for Nominations: 2010 CoMSEF Graduate Student Awards

CoMSEF is soliciting nominations for the 2010 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 2010 awards will be presented at the Annual Meeting in Salt Lake City.

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, Clare McCabe (c.mccabe@vanderbilt.edu), by October 1, 2010.



In addition, nominees must submit an abstract to the CoMSEF Poster session. The deadline for submission of poster abstracts is May 3rd, 2010.

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 Clare McCabe (c.mccabe@vanderbilt.edu) if you have questions about the award.

Research Highlight: Self-Assembly of Symmetric Diblock Copolymers in Planar Slits with and without Nanopatterns

By: Coray M. Colina

Although computational power is constantly increasing, fully atomistic approaches are still prohibitive when studying many phenomena. Coarse-grained models have allowed for the simulation of polymers (Glotzer and Paul, Annu. Rev. Mater. Res., 2002, 32401-32436), biological systems (Voth, G. A., "Coarse-Graining of Condensed Phase and Biomolecular Systems" CRC Press, 2008), and a plethora of diblock copolymer systems confined between planar surfaces (Petrus, et. al. Langmuir 2010, 26, 3695-3709), among many others.

The Dissipative Particle Dynamics (DPD) method has been exploited recently by Petrus, Lísal and Brennan (Langmuir 2010, 26, 3695-3709) to explore the spontaneous nanostructure formation of symmetric diblock copolymers confined between planar surfaces both with and without nanopatterns. The authors performed a systematic study of a generic model that might represent a low molecular weight PS-PVP copolymer at a given temperature. Several nanopatterned slits were considered with blueprints of different slit widths and surface patterns to investigate the competing effects of physical adsorption and confinement on the copolymer self-assembly. Petrus et al. show in this study how coarse-grained methods, in this case the DPD technique, are able to capture the strong influence of nanopatterns on copolymer conformational and adsorption behavior, as well as the ability of the copolymer to recognize different surface motifs. The authors have also recently written a book chapter entitled "An Introduction to Coarse-Graining Approaches: Linking Atomistic and Mesoscales" directed towards the novice (and not so novice) modeler. The chapter will appear this year, in the book entitled "Process Systems Engineering: Vol. 6 Molecular Systems Engineering" edited by Claire Adjiman and Amparo Galindo from Imperial College, WILEY-VCH Verlag GmbH & Co.

This work begins to pave the way to facilitate an understanding of the fundamental physics that occurs when diblock copolymers are confined in planar slits. Moreover, the opportunities follow to exploit this technique for applications to sensors, microelectronics, drug delivery, and biomaterials.

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!

Research Highlight: Computation-aided design of metal-organic frameworks for separations

By: J. Ilja Siepmann

One of the primary applications for nanoporous materials is the separation of complex gas mixtures that allows for an enrichment of desirable compounds from a feed stream through selective adsorption. Due to the nanoscale nature of the pore structures, the adsorption mechanism involves a complex interplay of enthalpic and entropic effects. In addition, kinetic control (selective diffusion) is another mode for separation in porous materials. There is considerable difficulty in probing the molecular-level detail of the adsorbate-adsorbent interactions by experimental means and, hence, molecular simulation has greatly contributed to understanding and predicting adsorption in nanoporous materials. Most of the previous simulations have investigated the adsorption of neat hydrocarbons or mixtures containing a few hydrocarbons in rigid sorbent materials. Recent work by Randy Snurr's group [Dubbeldam *et al.*, Separation and Molecular-Level Segregation of Complex Alkane Mixtures in Metal-Organic Frameworks, *JACS* **2008**, *130*, 10884] expands upon this by investigating the selective adsorption of a 13-component mixture (in the C_5 – C_7 range) in a metal-organic framework (MOF), a new class of molecular adsorbents with tailorable channels. The authors show that a specific MOF exhibits high adsorption selectivity for normal and monobranched alkanes and, hence, can enhance the concentration of more highly branched alkanes in the exit stream, thereby boosting the research octane number and fuel quality. More recently, this group has developed techniques to predict the adsorbate-induced structural changes in MOFs [Dubbeldam *et al.*, Method for Analyzing Structural Changes of Flexible Metal-Organic Frameworks Induced by Adsorbates, *JPCC* **2009**, 19317]. These papers will spark considerable interest in the development of novel MOFs that exhibit even more advantageous adsorption selectivity for hydrocarbon mixtures or larger storage capacities.

ChEnected

ChEnected—Where Chemical Engineers Mix it Up—is a unique online community created for and by young professional chemical engineers. Presented by AIChE, ChEnected is where chemical engineers can read, view, contribute, and engage with everything Chem-E. Learn new skills, solve challenges, find mentors, engage with other chemical engineers, and gain more exposure to hiring companies.

Visit http://chenected.aiche.org/

Annual Meeting Sessions

CoMSEF will sponsor or co-sponsor 28 sessions at the 2010 AIChE Annual Meeting in Salt Lake City, November 7-12. In addition to the many sessions that CoMSEF regularly (co-)sponsors, there are a few new sessions at the upcoming meeting. Proposals to present should be submitted on the web by: Monday, May 3, 2010 at 11:59pm (EST)

Happy Birthday, Prof. Sandler!!
We are pleased to co-sponsor sessions in honor of Professor Stanley Sandler's 70th birthday.

Simulation Based Engineering and Science Topical
CoMSEF will co-sponsor a Topical Summit on Simulation Based Engineering and Science (SBE&S), which will consider the implications of SBE&S for science and industry including key technological and applied capabilities and their impacts, the workforce, education, national investment and policy and the role of the Institute.

Wednesday CoMSEF Plenary Session
This year marks the inaugural year of the CoMSEF Plenary session, which will feature an invited presentation by the first CoMSEF Early Career award winner, Professor Ed Maginn.

Students and Advisors: Don't Forget the Monday Evening Poster Session!
A yearly highlight is the CoMSEF Poster Session, where the CoMSEF Graduate Student Award winners are selected. The awards recognize excellence in research by graduate students in the field of computational molecular science and engineering. Awardees are selected on the basis of a nomination letter from their advisor (who must be a member of CoMSEF), their CV, and their poster presentation.

Annual Meeting Sessions

Co-Sponsor	Session
10,18j	Workshop On National Investment, Policy and Education in Simulation-Based Engineering and Science
10,18j	The Application of Simulation Based Engineering and Science to Industrial Operations and Engineering Management of Enterprise Process Systems: Invited Speakers
10,18j	Innovation and Insight Via High Fidelity Simulation and Large Database Studies of Micro, Macro and Multi-Scale Phenomena: Invited Speakers
1a	In Honor of Stanley Sandler's 70th Birthday I and II
	Plenary Session on Computational Molecular Science and Engineering
	CoMSEF Poster Session
	Recent Advances in Molecular Simulation Methods I and II
15c	Molecular Modeling of Biophysical Processes I - Molecular
15c	Molecular Modeling of Biophysical Processes II - Multiscale
	First-Principles Simulations of Condensed Phases
	Chemistry and Kinetics Integrated CFD Modeling
8e	Computational Studies of Electronic and Photonic Materials
	Industrial Applications of Computational Chemistry and Molecular Simulation I and II
10d	Multiscale Modeling
10d	Multiscale Modeling II: Materials Processing
8a	Modeling and Simulation of Polymers
2e	Molecular Simulation of Adsorption I and II
1a	Computational Studies of Self-Assembly
1a	Development of Intermolecular Potential Models
20,1g	Computational Catalysis I, II, and III
10d	Numerical Methods for Molecular and Mesoscopic Systems
	The Industrial Fluid Properties Simulation Challenge