Computational Molecular Science and Engineering Forum

for the combined community of engineers and scientists developing and applying molecularly based theories, modeling, and simulation

CoMSEF Newsletter

AIChE

Graduate Student Awards

CoMSEF recently solicited nominations for the inaugural CoMSEF awards to recognize 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 a $500 honorarium. Two awards will be given annually and will be funded by the recently-instituted $5/yr membership dues. The 2006 awards will be presented at the CoMSEF plenary session (session number 21000) at the AIChE Annual Meeting.

Nominations consisted of a nominating letter from the student's research advisor and the curriculum vitae of the nominee. Due on August 1, 2006, 11 nominations were received by the CoMSEF chair. Nominees must present a poster at the CoMSEF Poster session (session number 21004) and must be a graduate student at the time of the poster presentation (the faculty nominator must be a member of CoMSEF). Award recipients will be selected from the nominations by a committee composed of CoMSEF officers based on the student's CV, the nomination letter from the advisor, the quality of the poster, and the student's ability to describe the poster work.

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In This Issue

Highlights of FOMMS 2006

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The conference co-chairs, senior advisors, and several members of the programming committee.

The application of molecular modeling and simulation technologies not only advances the fundamental chemical and materials sciences but also increasingly impacts the chemical, materials and pharmaceutical industries. Modeling and simulation includes the whole range of tools from first-principles electronic structure methods (quantum chemistry and density functional methods) to atomistic simulation (molecular dynamics and Monte Carlo methods), mesoscale methods (field theoretic and particle-based coarse-grained methods), and molecular level theoretical approaches. More and more, the information supporting the improvement of product and process discovery, development and design comes from fundamental computation.

In view of the growing importance of modeling and simulation, the Molecular Modeling Task Force of CACHE (http://www.che.utexas.edu/cache/) initiated a conference series, the Foundations of Molecular Modeling and Simulation (FOMMS), to showcase the applications and development of computational quantum methods, molecular science, and engineering simulation. Two very successful FOMMS conferences were held at Keystone Resort, Colorado in July of 2000 and 2003.

Like its predecessors, FOMMS 2006 was a scientific meeting balanced between the methods of quantum mechanics, atomistic simulation, mesoscale methods and beyond, with application areas in chemistry, biology, materials and their respective industries. As with any successful conference series, the current set of topics represents an evolution over previous conferences.

In particular, a specific industrial applications session has been removed in favor of industrial presentations scattered throughout the program and new sessions on Nanoscience & Nanotechnology and Education have been added.

One of the important aims of FOMMS 2006 was to bring together and foster interactions among innovators (primarily academics including students and young faculty), researchers (developers of new methods for molecular simulation and computational chemistry), providers (vendors of hardware and software for molecular chemistry), and consumers, (primarily industrial users of the tools). Invited plenary speakers discussed a wide variety of theoretical and applied topics in talks that survey the field and highlight breaking trends. Two poster sessions provided opportunities for attendees to present their work. The schedule provided large blocks of time for informal discussions, relaxation, or leisure, as well as several receptions to facilitate interac-

tion between conference participants. The expectation is that scientific contributions presented at this conference stimulate innovation in advanced molecular modeling, computational science, and engineering simulation.

Manuscripts associated with both oral and poster presentations at the conference will again be considered for publication in special issues of Molecular Physics and Molecular Simulation. The quality and timeliness of the FOMMS papers is evidenced by the fact that more than half of the ten most downloaded papers from Molecular Physics in 2004 were papers from FOMMS 2003, including the single most downloaded paper.

We are very happy to report that FOMMS 2006 attracted over 125 participants (and 9 guests); 93 academic, 24 industrial, and 8 government lab. Although (as usual) Americans dominated the meeting (71), international participation was very high, especially from the UK (12) and Japan (11); Germany (5), Belgium and Netherlands (4), Australia, Denmark, France, Republic of Korea (2), and one (1) from Brazil, Canada, China, Croatia, Czech Republic, Iran, Italy, Poland, Russia, and Ukraine. These numbers brought in a healthy diversity of research interests and conversations were lively!

Initial feedback from the meeting's delegates indicates that sessions were very well-received, relevant to their work, and worth the time and effort of attendance. Overall, the speakers were excellent and many stayed a good portion of, if not the entire, week making follow-up conversation easier. Of special note is the overwhelming response that enough time was left for questions at the end of talks or during the panel discussions. Since promoting interaction and communication was an essential goal for FOMMS 2006, as organizers, we are especially proud of that result!

The task of reviewing the manuscripts for publication in special issues of Molecular Physics and Molecular Simulation has begun. In this regard FOMMS 2006 was also very successful, (to date) receiving 12 (out of 21) invited speaker manuscripts and 54 (out of 89) contributed poster manuscripts.

Since FOMMS 2006 participants expressed a very high interest in attending FOMMS 2009, plans are already underway on it's agenda. "Watch this space!"

FOMMS 2006 is organized under the auspices of the non-profit educational foundation CACHE Corporation in collaboration with the Computational Molecular Science and Engineering Forum (CoMSEF) of the American Institute of Chemical Engineers. We acknowledge financial support from, and express our gratitude to, the Department of Energy, BP, CULGI, Colorado School of Mines, Taylor & Francis, Accelrys, EniTechnologie, ExxonMobil, PPG Industries, Wavefunction, Vanderbilt University, and CACHE Corporation. Heartfelt appreciation is extended to all the invited speakers, the authors of the contributed papers, and the session chairs. We gratefully appreciate the energy and suggestions of Petr Kolar (Mitsubishi) in the early stages of FOMMS 2006 planning. Special thanks go to our Scientific Organizing Committee (see Table 1) for agenda and speaker suggestions as well as efforts in "advertising" the meeting. The success of FOMMS 2006 is mainly the result of the dedicated efforts of these individuals.

If you have any questions or additional comments, don't hesitate to send an Email. Additional information on FOMMS 2006 can be found at the website: www.fomms.org.

Table 1. Scientific Organizing Committees

Senior Advisors:
Peter T. Cummings, Vanderbilt University
James F. Ely, Colorado School of Mines
Phillip R. Westmoreland,
University of Massachusetts Amherst/NSF

Programming Committee:
Anne M. Chaka, National Institute of Standards and Technology
Kenneth A. Dill, University of California San Francisco
Johannes G.E.M. Fraaije, Universiteit Leiden, The Netherlands
Alain Fuchs, Université de Paris-Sud, France
Peter A. Gordon, ExxonMobil
Catherine T. Hunt, Rohm and Haas
David A. Kofke, University at Buffalo
Ronald G. Larson, University of Michigan
Jonathan D. Moore, The Dow Chemical Company
Matthew Neurock, University of Virginia
Jeffrey A. Nichols, Oak Ridge National Laboratory
John P. O'Connell, University of Virginia
Susumu Okazaki, Institute of Molecular Science, Japan
Costas C. Pantelides, Imperial College, London, UK
Doros N. Theodorou, National Technical University of Athens, Greece

Spring 2008 AIChE and ACS Meetings

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-sponsoring 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 very much in the formative stages, but we will likely co-organize two to three topical sessions in areas such as "Computation of Solid and Fluid Phase Equilibria," "Modeling of Aqueous Solutions," and "Computational Evaluation of Rate Constants." Suggestions for topics or volunteers to co-organize sessions are encouraged to contact Bill Schneider at: wschneider@nd.edu or (574) 631-8754.

CoMSEF General Meeting in San Francisco

CoMSEF will hold its annual General Meeting during the Fall 2006 AIChE Meeting. The meeting will be held jointly with Area 1a (Thermodynamics and Transport Properties) on Wednesday November 15 from 6-7 p.m. Look for the room number in the material handed out at the meeting. All CoMSEF members are invited to attend.

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
- Science Talk (Scientific American)
- NewScientist.com podcast

New CoMSEF Web Site

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

Though currently rather "bare bones," 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 Carol Hall in San Francisco

Two special sessions will be held at the Fall 2006 AIChE meeting in honor of Carol Hall's 60th birthday and in recognition of her contributions to chemical engineering. The sessions will consist of invited talks from Carol's colleagues and students. For detailed information regarding the sessions, see the links below.

CoMSEF Sessions for Fall 2006 AIChE Mtg.

Information regarding the CoMSEF sessions for the Fall 2006 AIChE meeting in San Francisco is available on the web. Here are the links:

- Plenary Session on Computational Molecular Science and Engineering
- Graduate Student Award Poster Session
- Carol in Thermoland I: A Session in Honor of Carol Hall's 60th Birthday
- Carol in Thermoland II: A Session in Honor of Carol Hall's 60th Birthday
- Industrial Applications of Computational Chemistry and Molecular Simulations I
- Industrial Applications of Computational Chemistry and Molecular Simulations II
- The Third Industrial Fluid Properties Simulation Challenge
- Development of Intermolecular Potential Models
- Best Practices in Electronic Structure Calculations
- Multiscale Modeling I
- Multiscale Modeling II
- Recent Advances in Molecular Simulation Methods
- Algorithms, Applications, and Best Practices in Parallel and Grid Computing
- Numerical Methods for Molecular and Mesoscopic Systems
- Nucleation and Growth
- Computational Studies of Self-assembly I
- Computational Studies of Self-assembly II
- Multiscale Modeling and Characterization of Polymers
- Structure and Properties of Polymers III: Dynamics of Glass Formers
- Transport in Nanoporous Materials
- Molecular Modeling of Fuel Cells and Electrochemical Systems I
- Molecular Modeling of Fuel Cells and Electrochemical Systems II
- Molecular Modeling of Fuel Cells and Organic-Semiconductor Systems
- Computational Biology: Systems Modeling I
- Computational Biology: Systems Modeling II
- Computational Biology: Proteins and DNA
- Computational Biology: Membrane Phenomenology
- Computational Genomics
- Computational Catalysis I
- Computational Catalysis II
- Computational Catalysis III
- Molecular Modeling in Electronic Materials Processing

News Briefs

- **Industrial & Engineering Chemistry Research**: **Eduardo Glandt Festschrift** (link to more)
- **DOE Seeks Proposals to Use INCITE Resources**: "Secretary of Energy Samuel W. Bodman has announced that the U.S. Department of Energy's Office of Science is seeking new proposals to support innovative, large-scale computational science projects…" (link to more) (link to DOE INCITE web site)
- **DOE Announces $60 Million in New SciDAC Awards**: "The projects are aimed at accelerating research in designing new materials, developing future energy sources, studying global climate change, improving environmental cleanup methods and understanding physics from the tiniest particles to the massive explosions of supernovae. (link to more) (link to SciDAC's web site)
- **IBM to Build Cell-Based Supercomputer for Los Alamos**: "The U.S. Department of Energy's National Nuclear Security Administration (NNSA) has selected IBM to design and build the world's first supercomputer to harness the power of the Cell Broadband Engine (Cell B.E.) processor aiming to produce a machine capable of a sustained speed of up to one petaflop." (link to more)
- **Technology Review's 10 Emerging Technologies**: "This year our list of technologies that are worth keeping an eye on is particularly wide ranging—but all of our picks are ready to have a big impact on business, medicine, or culture…" (link to more)
- **The Economist: Computing the future**: "The practice of science may be undergoing yet another revolution…" (link to more) (link to the Towards 2020 Science web site)
- **Cray's Adaptive Supercomputing - A Paradigm Shift**: "Adaptive supercomputing will cause a paradigm shift in the way users select and use HPC systems...The Cray motto is: adapt the system to the application - not the application to the system…" (link to more)
- **Japan Bests IBM in Supercomputer Stakes**: "For those of you keeping score out there, Japan is about to take back the world speed record for computing it held earlier in the decade. The MDGrape-3 at Riken (formerly known as the Institute of Physical & Chemical Research) in Yokohama was clocked at a mind-boggling one quadrillion calculations per second…" (link to more)
- **CSE-Online 1.0**: "[Computational Science and Engineering 1.0]...is now available with more than 30 applications to choose from." (link to more)
- **MIT's Energy 'Manhattan Project'**: "Scientists at MIT are undertaking a big, ambitious, university-wide program to develop innovative energy tech under the auspices of the school's Energy Research Council…" (link to more)
- **Cray Wins $52M Supercomputer Contract with DOE's NERSC**: "Cray Inc. and the U.S. Department of Energy (DOE) Office of Science announced on Thursday that Cray has won the contract to install a next-generation supercomputer at the DOE's National Energy Research Scientific Computing Center (NERSC). The systems and multi-year services contract, valued at over $52 million, includes delivery of a Cray massively parallel processor supercomputer, code-named "Hood."…" (link to more)
- **Chemistry Central**: "Chemistry Central is a new service publishing peer-reviewed open access research in chemistry from BioMed Central, the leading biomedical open access publisher." (link to more)
- **Top hydrogen-storing polymer revealed**: "A series of computer simulations has identified a polymer material with a very large capacity for storing hydrogen that could be exploited in fuel cells…" (link to more)
- **U.S. supercomputer gets speedier**: "The most powerful supercomputer available for general scientific research in the United States has doubled its speed, officials said Friday. The 54-cabinet Cray XT3 supercomputer at Tennessee's Oak Ridge National Laboratory has been upgraded from 25 teraflops to 54 teraflops, or 54 trillion mathematical calculations per second, they said…" (link to more)
- **Sales method pays off for materials scientists**: "The same computer methods used by online sales sites to suggest books to customers can help predict the crystal structures of materials…" (link to more)
- **Nanoparticles By Design**: "Simulations predict wide range of geometries possible via polymer grafting…" (link to more)
- **Technology Review's 2006 Young Inventors Under 35**: "Since 1999, the editors of Technology Review have honored the young innovators whose inventions and research we find most exciting; today that collection is the TR35, a list of technologists and scientists, all under the age of 35. Their work--spanning medicine, computing, communications, electronics, nanotechnology, and more--is changing our world…" (link to more)
- **Folding@Home PS3 client announced**: "Today in Germany, Sony demoed their Folding@Home client for the PS3...Using the Cell processor of the PS3, we should be able to do more folding than what one could do on a PC. Also, since the PS3 has a powerful GPU, the PS3 client will offer real time visualization for the first time." (link to more)
- **Hybrid Particle-Field Simulations of Polymer Nanocomposites**: "We present a theoretical framework and computer simulation methodology for investigating the equilibrium structure and properties of mesostructured polymeric fluids with embedded colloids or nanoparticles.." (link to more)
- **Mechanisms of the Wurtzite to Rocksalt Transformation in CdSe Nanocrystals**: "We study the pressure-driven phase transition from the four-coordinate wurtzite to the six-coordinate rocksalt structure in CdSe nanocrystals with molecular dynamics computer simulations…" (link to more)
- **Influence of Confinement on the Fragility of Antiplasticized and Pure Polymer Films**: "We investigate by molecular dynamics simulation how thin film confinement modifies the fragility of a model glass-forming liquid characterized previously in the bulk…" (link to more)
- **High-Pressure Phases of Silane**: "High-pressure phases of silane SiH_{4} are predicted using first-principles electronic structure methods…" (link to more)