Highlights of FOMMS 2006

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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 interaction 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 is almost complete. 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. As for the status of the special issues, 43 papers are completely reviewed, 17 for Mol. Phys. and 26 for Mol Sim. Nineteen papers are accepted so far and we are waiting on reviewers for a few manuscripts whilst the rest are with the authors for revision.

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

Figure 1. Members of the FOMMS-2006 Scientific Organizing Committee: From left, Joe Golab, Matt Neurock, Clare McCabe, Susumu Okazaki, Johannes Fraaije, Jim Ely, Phil Westmoreland, Jonathan Moore, David Kofke, Alain Fuchs, Jeff Nichols, and Peter Cummings