Fall 2007 Highlights

- Symposiums to Honor Bill Goddard's 70th Birthday, and memorials for Phil McGee and Robert Fenney
- Division's CCG Excellence Awards will be Presented to 5 Students
- Update on *Annual Report in Computational Chemistry* (ARCC)

COMP Newsletter

Statement from the Chair

Ralph A. Wheeler, COMP Chair 2007, reports on the division's status

I am pleased to report that the COMP Division continues as a financially strong and active division of the ACS and that the COMP leadership has begun implementing the Division's Strategic Plan to lead the innovative use of computers in experimental, theoretical and computational chemistry. The COMP Division's Strategic Plan was formulated by the Executive Committee at our annual strategic planning meeting in Spring 2007, assisted by professional facilitators from the ACS. Our goal was to develop a long-term view of the division's mission to make sure the COMP Division remains on track to becoming recognized as the world's premier computational chemistry community by 2009. The COMP Division's officers are committed to maintaining our foundation of robust scientific programs, while enhancing member services, outreach activities, and professional development. Our vision will be accomplished by (1) strengthening the community of computational chemists by providing opportunities for networking and career growth through enhanced outreach, (2) developing and delivering premier activities, products, and services for computational chemical research and education, and (3) refining divisional administration and implementing operational processes to use time and financial resources for enhanced member benefit.

To optimize member benefits by refining divisional administration, the COMP Division's Executive Committee is constantly examining duties of the various officers. The Committee is currently producing a procedures manual to ensure continuity when committee membership changes, modifying officer responsibilities to optimize efficiency, and establishing communication channels for regular reporting activities to promote best practices and continuity.

To strengthen the community of computational chemists, the COMP Division has started several new initiatives. First, the division initiated a program of mentoring lunches at the Spring 2007 national meeting, coordinated by Drs. Wendy Cornell and Rommie Amaro. The program provided a forum for two groups of students to ask questions of scientists employed in either industry or academia in an informal lunch setting. The program provided a wonderful opportunity for students to network and cost the division nothing because Glaxo-Smith-Kline generously provided funds for the industrial lunch. The Executive Committee is currently evaluating the program and deciding how to improve it. In addition, the division conducted electronic elections for the second year in a row and, once again, we experienced unprecedented participation. Please join me in thanking Dr. Lisa Balbes for running our elections and congratulating her for a job well done. Thanks to Lisa's efforts, the COMP Division is once again at the forefront of the ACS in using electronic technologies and, in fact, the ACS is presenting our experience as a model for other divisions to move their elections online. In the near future, the COMP Division's leadership will further strengthen our use of electronic information delivery by evaluating and revising the division's website.

To continue developing and delivering premier activities, products, and services for computational chemical research and education, the COMP Division continues robust programming at national meetings under the able leadership of the Program Chair, Professor Jeffry Madura, and provides unprecedented member access to some of the world's uniquely valuable computational chemistry literature. In this issue of the COMP newsletter, you will read about a number of exciting technical symposia planned for future national meetings, as well as the activities of our incredibly generous corporate partners (see http://membership.acs.org/C/COMP/ for a complete list). Volume 3 of *Annual Reviews in Computational Chemistry* (ARCC), edited by Drs. David Spellmeyer

and Ralph Wheeler, recently went to press and will soon show up in your mailbox. Volume 3 includes contributions in six topical subject areas—Biological Modeling, Physical Modeling, Quantum Chemistry, Chemical Education, Simulation Methodologies, and Emerging Technologies. The articles in each section provide concise summaries of their respective topics unavailable anywhere else. Invitations are currently being issued for Section Editors for Volume 4 and volunteers will soon be solicited to author articles. Anyone interested in contributing to the production of Volume 4 of ARCC should contact Ralph Wheeler or David Spellmeyer as soon as possible. In addition, the division is officially affiliated with the ACS *Journal of Chemical Theory and Computation* and *Journal of Chemical Information and Modeling*, as well as the Elsevier publication *Journal of Molecular Graphics and Modeling* (JMGM). Under the continuing leadership of its U.S. Editor, Andy Holder, JMGM has attained a steadily increasing flow of quality papers and a continuously improving impact factor. Members may also receive a discounted subscription to JMGM.

Ralph Wheeler

Symposia for Boston ACS Meeting

Highlights for Boston ACS Meeting and a preview of the New Orleans Meeting

The Fall 2007 meeting in Boston promises to be interesting, as a number of COMP symposium organizers have scheduled a variety of topics ranging from drug discovery to computational methodology.

- Recent Advances in Studies of Molecular Processes at Interfaces (Liem Dang)
- Bold Predictions in Theoretical Chemistry: A Symposium in Honor of One of the Boldest, Bill Goddard, on the Occasion of his 70th Birthday – oral and poster sessions (Emily Carter, Mark Gordon)
- Protein-Nucleic Acid Interactions: Experimental and Modeling Analysis (Rita Mihailescu)
- Current Techniques in Molecular Simulation of Biological Systems (Nitin Rathore)
- Computational Science & Engineering Advances Supported by NSF Resource (John Towns)
- Phil McGee Memorial Symposium: QSAR Reborn (John Block, Bob Clark)
- Emerging Technologies (Curt Brenneman)
- Poster Session
- CCG Excellence Award (Andrew Good)
- General Oral – Quantum Chemistry (Adrian Roitberg)
- General Oral – Molecular Mechanics (Emilio Esposito)
- General Oral – Drug Discovery (IracheVisiers)
- Antifreeze Proteins: A Memorial Symposium for Robert Fenney (Andrzej Wierzbicki)
- Evaluation of Computational Methods: Insights, Philosophies and Recommendations (Anthony Nicholls, Ajay Jain)

The poster session will take place on Tuesday night. The CCG Excellence Awards and HP Outstanding Junior Faculty Award will be presented at that time. The COMP division would like to acknowledge the generosity of our sponsors who provide funding for selected symposia and the poster session.

Looking further ahead to the Spring 2008 National American Chemical Society Meeting in New Orleans we will have the opportunity to do joint ACS-AIChe programming with the CoMSEF, the Computational Molecular Science and Engineering Forum part of AIChe. Discussions with the folks of CoMSEF have yielded several interesting symposia given below. If you have any ideas or would like to organize a symposium for the Philadelphia meeting (Fall 2008) please contact Jeffry Madura at madura@duq.edu.

- Computational Catalysis (A.M. Rappe)
- Computational Evaluation of Rate Constants (T.N. Truong)
- Computational Phase Equilibria (I. Siepmann)
- Drug Discovery (I. Visiers)
- Molecular Mechanics (E.X. Esposito)
- Molecular Modeling Applied on DPP-4 Inhibitor Programs (Y-D. Gao)
- Quantum Chemistry (A. Roitberg)
- Replica Exchange: New Methods & Applications to Protein Folding & Other Large Systems (S. Rick)
- Thomas Kuhn Paradigm Shift Award Competition (A. Nicholls)

Finally, this is a call for graduate students and post-doctoral Computers in Chemistry Division members to assist in chairing one or two General Oral sessions. If you are attending a National ACS meeting and would be willing to chair one or two of the General Oral half-day sessions, the COMP Division can arrange to have your registration for that meeting paid. You need to be an ACS member and a member of the COMP division. Please contact Dr. Madura for additional details.

ARCC update, Volume 3 coming soon

Annual Reports in Computational Chemistry to be published in Oct. 2007

Annual Reports in Computational Chemistry (ARCC) focuses on providing timely reviews of topics important to researchers in the field of computational

chemistry. The ARCC is published and distributed by Elsevier (edited by D. Spellmeyer and R. Wheeler) and is sponsored by the COMP division. We are very pleased that both Volumes 1 and 2 have received a very positive response from our readers. Volume 3 will be published in October and will be shipped to current COMP members as part of their membership benefits.

Table of Contents for ARCC, Volume 3:
Section 1: Simulation Methodologies
(Section Editor: C. Simmerling)

- "Molecular Simulations of pH-Mediated Biological Processes," J. Khandogin and C.L. Brooks, III
- "Extending Atomistic Time Scale Simulations by Optimization of the Action," A.S. Clarke, S.M. Hamm, and A.E. Cárdenas
- "Fishing for Functional Motions with Elastic Network Models," A.J. Rader
- "Alchemical Free Energy Calculations: Ready for Prime Time?" M.R. Shirts, D.L. Mobley, and J.D. Chodera

Section 2: Biological and Biophysical
(Section Editor: H. Carlson)

- "Linear Quantitative Structure-Activity Relationships for the Interaction of Small Molecules with Human Cytochrome P450 Isoenymes," T. Fox and J.M. Kriegl

Section 3: Chemical Education
(Section Editor: T. Zielinski)

- "Observations on Crystallographic Education," P.E. Fanwick
- "Achieving a Holistic Web in the Chemistry Curriculum," H.S. Rzepa

Section 4: Materials and Polymers
(Section Editor: J. Madura)

- "The Role of Long-Time Correlation in Dissipative Adsorbate Dynamics on Metal Surfaces," J.M. Moix and R. Hernandez

Section 5: Quantum Chemistry
(Section Editor: T.D. Crawford)

- "An Active Database Approach to Complete Rotational-Vibrational Spectra of Small Molecules," A.G. Császár, G. Czakó, T. Furtenbacher, and E. Mátyus
- "The Effective Fragment Potential: A General Method for Predicting Intermolecular Interactions," M.S. Gordon, L. Slipchenko, H. Li, and J.H. Jensen
- "Gaussian Basis Sets Exhibiting Systematic Convergence to the Complete Basis Set Limit," K.A. Peterson

Section 6: Emerging Technologies
(Section Editor: W. Cornell)

- "Principles of G-Protein Coupled Receptor Modeling for Drug Discovery," I. Visiers

HP Outstanding Junior Faculty Award Program

Sponsored by Hewlett-Packard

Hewlett-Packard and the ACS Division of Computers in Chemistry (COMP) were pleased to present four HP Outstanding Junior Faculty Awards that provided a $1,000 in travel funds to each of the four outstanding tenure-track junior faculty selected at the Spring 2007 ACS National Meeting.

The 2007 (Chicago) winners were:

Nathan Baker, Washington University, "Modeling membrane potentials: when does discreteness matter?"

Michael Feig, Michigan State University, "Implicit modeling of complex cellular environments"

George Kaminski, Central Michigan University, "Computing pKa shifts of turkey ovomuvoid third domain (OMTKY3) residues with a polarizable force field"

Ray Luo, University of California - Irvine, "Scaling in biomolecular hydration: A critical analysis of implicit solvents"

The Awards are designed to assist new faculty members in gaining visibility within the COMP community. While special consideration will be given to Assistant Professors presenting work in the area of algorithm and methods development, applications are invited from all current tenure-track junior faculty who are members of ACS and the ACS Division of Computers in Chemistry. Selection criteria will include the novelty and importance of the work to be presented.

To apply, an e-mail nominating one's self should be sent to Jeffry Madura.

Chemical Computing Group Excellence Award Recipients Announced

CHEMICAL COMPUTING GROUP
Scalable Software. Scalable Science.

CCG Excellence Awards Tuesday Evening

Chemical Computing Group (CCG) and the American Chemical Society's Division of Computers in Chemistry (COMP) are pleased to present five CCG Excellence Awards to outstanding graduate students, recognizing the quality and relevance of their research. The awards provide $1,150 for travel expenses to the Boston meeting and provide a one-year software license for the Molecular Operating Environment (MOE) (http://www.chemcomp.com/).

The awardees, in alphabetical order, are:

- James S. M. Anderson: "Novel basis-set free approaches to solving the electronic-Schrödinger equation", *McMaster University*
- Christina R. Crecca: "How much experimental data is needed to predict a protein's structure?", *University of Florida*
- Raed Khashan: "Development of scoring functions for protein-ligand binding based on frequent geometric and chemical patterns of inter-atomic interactions at their interfaces", *University of North Carolina*
- Lauren Wickstrom: "To be native or not to be native, that is the question: Studies of the unfolded state

structure of the Villin Headpiece Helical Subdomain", *Stony Brook University*

- Kai Zhu: "Improving generalized Born model in protein side chain and loop prediction", *Columbia University*

Applications for awards to attend the meeting in New Orleans, LA in March 2008 consist of an extended abstract, CV, personal statement, and a supporting letter from the student's advisor and are due to Andrew Good, andrew.good@bms.com (electronic format is preferred). In addition, an abstract for the scientific presentation must be submitted in the CCG awards COMP section of the ACS OASYS system (http://oasys.acs.org/oasys.htm) for online submissions prior to the deadline for the meeting at which the awards will be presented. Submissions are restricted to North, Central and South American students. Please see the COMP website for more details.

Cheminformatics Award for Young Researcher

Applications Invited for CSA Trust Jacques-Émile Dubois Grant for 2007

The Chemical Structure Association (CSA) Trust has a grant program in the area of cheminformatics in honor of Professor Jacques-Émile Dubois. Each year grant is awarded to provide funding for the career development of young researchers (under age 35) who have demonstrated excellence in their education, research or development activities that are related to the systems and methods used to store, process and retrieve information about chemical structures, reactions and compounds. A Grant will be awarded annually up to a maximum of US $3,000.

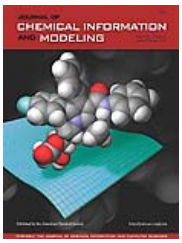
For more information please visit http://www.csa-trust.org/.

Journal of Molecular Graphics and Modelling

The *Journal of Molecular Graphics and Modelling* (JMGM) is doing great! We have a steady and increasing stream of manuscripts, and have become increasingly selective in the quality of papers published. The *Journal* is healthy and widely cited. Our impact factor (an index of citations to articles in the journal) has been steadily increasing over the past several years. As always, we find our connection with COMP to be beneficial, and we solicit your submissions.

Andy Holder, U.S. Editor, *JMGM*

JCTC and JCIM



The COMP division has partnered with ACS publications and affiliated with the *Journal of Chemical Theory and Computation (JCTC)* and the *Journal of Chemical Information and Modeling* (JCIM) to provide a focal point for publications based on new theories, methodology, and/or important applications in quantum chemistry, molecular dynamics, statistical mechanics and chemical informatics. Both journals are edited by William L. Jorgensen at Yale University.

In its first year of receiving an impact factor, *JCTC* ranked in the top 20 in Multidisciplinary Chemistry with an impact factor of 3.627. It received 647 citations in 2005 – an increase of 553% over the previous year.

In the category of computer science, information systems, *JCIM* ranks #2 in citations with 7,026 total cites out of 87 journal in that category. The journal received an impact factor of 3.423.

Emerging Technologies Award

$1000 prize to be awarded at the Boston ACS national meeting

The COMP Division of the ACS will hold the eighth annual Symposium on Emerging Technologies in Computational Chemistry at the American Chemical Society National Meeting, Boston, MA, August 19-23, 2007. The objective of the symposium is to stimulate, reward, and publicize major methodological advances in computational chemistry.

The talks will be evaluated by a Panel of Experts on the quality of the presentation and the impact that the research will have on the future of computational chemistry and allied sciences. The symposium is ideal for presenting your latest and best research on new techniques, applications and software development. Schrödinger, Inc. sponsors the $1,000 award for the best talk at the symposium.

All are invited to participate. To enter the competition, you should submit a regular short ACS abstract via http://oasys.acs.org/ prior to the OAsys deadline. It is also necessary to email a long (~1,000-word) abstract to Curt Breneman. The presentations must be original, novel and concise. After receipt, the long abstracts will be evaluated by experts to determine which individuals will be selected to give oral presentations at the symposium. Finalists will be notified well in advance of the meeting. Presentations submitted through OAsys that cannot be part of the Emerging Technologies Symposium will be rescheduled in another appropriate COMP session at the Boston meeting.

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