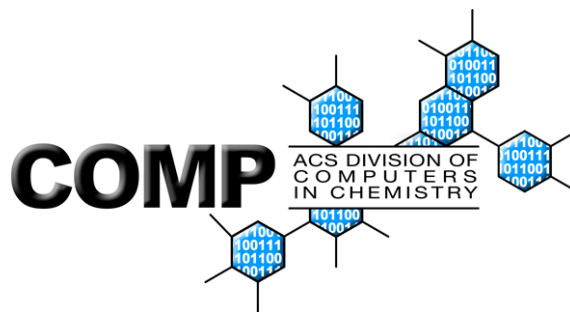


Spring 2007 Highlights

- Symposia to Honor Barry Honig's 65th Birthday and Yvonne C. Martin
- Emily Carter to be Honored Tuesday Afternoon with the ACS Award for Computers in Chemical & Pharmaceutical Research
- Division's CCG Excellence Awards will be Presented to 5 Students



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 is a strong and vital division of the ACS and the leadership continues looking for ways to better serve the membership. The COMP Division's Executive Committee met in Washington DC this past February for the division's annual Strategic Planning Meeting, assisted for the first time 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. Current activities directed toward these goals include continued robust

programming at national meetings under the able leadership of the Program Chair, Jeffry Madura, continuing commitments from our corporate partners to sponsor the COMP Division's various award programs, and unprecedented member access to some of the world's uniquely valuable computational chemistry publications.

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 corporate partners. First, Chemical Computing Group has generously agreed to continue sponsorship of the CCG Excellence Awards for graduate student travel (<http://www.chemcomp.com/>). The program supports five graduate student travel awards per national meeting. Each student awardee will receive a check for \$1,150 to support travel to attend the national meeting and present research results as part of the COMP Division's technical program. In addition, each awardee's research advisor receives a one-year license for the Molecular Operating Environment (MOE) software for research and teaching purposes. Please note that the deadline for applications is usually several weeks before the normal COMP deadline for abstract submission for each national meeting. Andrew Good, CCG Excellence Awards Coordinator, is managing the review of applications and may be contacted with any questions. The awards

provided by the CCG are an outstanding benefit to our younger members and we are extremely grateful to CCG for their continued support of the program. Second, Accelrys has generously agreed to continue their support of the COMP Division by sponsoring the ACS Award for Computers in Chemical and Pharmaceutical Research. This year's winner, Professor Emily Carter of Princeton University, will continue the tradition established by Accelrys and present her award address as part of a COMP Division symposium in her honor. Additionally, Hewlett-Packard has pledged continued support for the HP Outstanding Junior Faculty Award Program. This program honors four outstanding tenure-track junior faculty by providing each with an HP Outstanding Junior Faculty Award and \$1,000 in travel funds to attend the national meeting and present research results as part of the COMP Division's technical program. Application materials described within this newsletter should be sent to the award coordinator, Jeffry Madura. On behalf of the entire COMP Division membership, I want to thank all of our corporate sponsors, including those listed above, for their generous support of the division's activities.

One of the biggest benefits brought to the COMP membership over the past several years is access to some of the world's premier computational chemistry literature. The division is now 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 2005 impact factor (2.33) approaching that of *Chem. Phys. Lett.* (2.43). Members may also receive a discounted subscription to JMGM. One of the most exciting developments for the COMP Division was the successful launch of *Annual Reports in Computational Chemistry* (ARCC). Under the superb leadership of the Editor, David Spellmeyer, the first two volumes were delivered to members in 2005 and 2006. This year, Volume 3 will head to the publisher shortly after the Chicago national meeting and should arrive in members' mailboxes later in 2007. Volumes 3 and 4 will be co-edited by David Spellmeyer and Ralph Wheeler and Volume 3 includes contributions in six topical subject areas—Biological and Biophysical, Chemical Education, Emerging Technologies, Materials and Polymers, Quantum Mechanics and Simulation Methodologies. We anticipate that Volume 3 will include 12-15 articles providing concise summaries of their respective topics unavailable anywhere else. COMP Division members will especially appreciate the cumulative index for all volumes that will enable long-time members to locate all summaries of a given topic in any of their collected volumes quickly and easily. If you would like to contribute as an author in Volume 4, please contact Ralph or David as soon as possible.

In addition to our current activities, the Executive Committee is constantly searching for new ways to add value to membership in the COMP Division. Last year, we analyzed results of an on-line survey and found that more than 30% of division members would like to see (1) more electronic communication, (2) more graduate awards and (3) more divisional involvement at regional and local levels. During our long-range Strategic Planning Meeting, we considered your wishes in drafting the COMP Division's Strategic Plan, but we will need your input constantly, throughout the process of

refining and implementing the plan. Specifically, the Executive Committee will soon release a Draft Strategic Plan, along with an invitation for members to add value with positive suggestions. In the meantime, keep an eye on your email "In" box for communications from the division, monitor the COMP website

(<http://membership.acs.org/C/COMP/>) for new information, and email an officer with your best ideas. We need your help to make the COMP Division the world's premier computational community. Remember, there is no community without you!

Ralph Wheeler

Symposia for Chicago ACS Meeting

Highlights for Chicago and preview of the Boston ACS Meeting

The Spring 2007 meeting in Chicago promises to be interesting, as a number of COMP symposium organizers have scheduled a variety of topics ranging from drug design to computational methodology. The symposia are:

- De Novo Design Coupled to Synthetic Feasibility
- Barry Honig 65th Birthday Symposium: Biological Applications of Implicit-solvent Models
- Computer Assisted Drug Design: Reminiscing about the Future, A Symposium Honoring Yvonne C. Martin
- Thomas Kuhn Paradigm Shift Award Competition
- ACS Awards Symposium in Honor of Emily Carter
- General Oral – Quantum Chemistry
- General Oral – Molecular Mechanics
- General Oral – Drug Discovery

The poster session will take place as usual on Tuesday night. The CCG sponsored Excellence awards will be presented to the students 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.

A number of symposia are in place for the Fall 2007 meeting in Boston. Please contact Jeffry Madura if you are interested in organizing a symposium. OASYS abstract submission is open through April 2, 2007. Symposia scheduled for the Fall 2007 meeting include:

- 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 on QSAR (John Block, Bob Clark)
- Emerging Technologies (Curt Brennenman)
- 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)

ACS Award for Computers in Chemical & Pharmaceutical Research

Sponsored by Accelrys

Professor Emily Carter of Princeton University is the winner of the 2007 ACS Award for Computers in Chemical and Pharmaceutical Research for her contributions to the fields of surface and materials science.

Carter received her B.S. degree at the University of California, Berkeley and her Ph.D. degree from the California Institute of Technology. After postdoctoral work at the University of Colorado, Boulder, Carter joined the faculty at the University of California, Los Angeles for 16 years until she moved in 2004 to her current appointment as a Full Professor in Mechanical and Aerospace Engineering and Applied Computational Mathematics at Princeton University.

Professor Carter will present her award address “Synergy in computational science and engineering” before the COMP Division on Tuesday morning. This award is generously sponsored by Accelrys.

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 ACS National Meeting in San Francisco.

The 2006 winners were:

Hendrik Heinz, University of Akron, Department of Polymer Engineering, “Force Fields for Inorganic Components in Hybrid Systems”

David van der Spoel, University of Uppsala, Department of Cell and Molecular Biology, “Protein Folding Properties from Molecular Dynamics Simulations”

Henryk Witek, National Chiao Tung University, Department of Applied Chemistry, “Relativistic parameterization of the SCC-DFTB method”

Anatoly Ruvinsky, University of Kansas, Center for Bioinformatics, “Novel statistical-thermodynamic method for computation of protein-ligand binding entropy: docking test with 11 scoring functions”

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 Jeffrey Madura.

Chemical Computing Group Excellence Award Recipients Announced



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 subsidize travel expenses to the Chicago meeting and provide a one-year software license for the CCG Molecular Operating Environment (MOE) (<http://www.chemcomp.com/>).

The awardees, in alphabetical order, are:

- Billy Griffin: “Neural network and ab initio studies of metal hydride nanoparticles,” *University of Arkansas*
- Maricris Lodrighito: “Externally corrected coupled-cluster methods employing method of moments of coupled-cluster equations and multi-reference perturbation theory,” *Michigan State University*
- Salma B. Rafi: “Molecular dynamic simulations help capture TB-drug-design’s most wanted: Mechanism of active site loop ordering,” *Stony Brook University*
- Sigifredo Sanchez-Carrera: “Electron-photon coupling in organic semiconductors: A DFT-based approach,” *Georgia Institute of Technology*
- Laura Thomas: “Monte Carlo investigations of fundamental properties of organic molecules in the gas and liquid phases,” *Yale University*

Applications for awards to attend the meeting in Boston, MA in August 2007 consist of an extended abstract, CV, personal statement, and a supporting letter from the student’s advisor and are **due to Andrew Good by April 6, 2007**. 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.

Join the COMP Division

Become a new COMP Division member or change your membership status by using the on-line form or calling 800.333.9511.

Membership dues are:

ACS Member \$15.00

Student Member \$7.50

Retiree \$15.00

Division Affiliate \$17.00

National Affiliate \$17.00

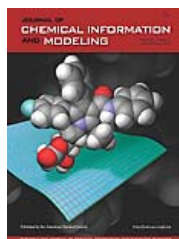
Outside US, add \$3.00 for postage

Join the COMP division!

<http://membership.acs.org/C/COMP/>

Go to COMP's website to obtain the most complete, up-to-date information available on events, publications and topics within the COMP division.

JCTC, JCIM, and JMGM



The COMP division is 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.

Comp members are encouraged to use JCTC, JCIM and JMGM as a forum for their publications. Articles describing research of substantial merit are invited. For more detailed information on JCTC and JCIM please visit the ACS publications website, <http://pubs.acs.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 submissions. The Journal is healthy and widely cited. We are pleased to be one of the journals that COMP is associated with, and solicit your submissions.

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

COMP website continuously improving

The COMP website now has its own RSS feed. In addition the website also features two employment related feeds. These feeds search the cen-chemjobs database and return currently open positions in computational chemistry, informatics, and information science. Visit the COMP website for more details at:

<http://membership.acs.org/C/COMP/>.

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