Fall 2008 Highlights

- COMP division elections from Aug. 8 to Sept. 19, 2008
- Division's CCG Student Excellence Awards and HP Outstanding Junior Faculty Awards will be Presented On Tuesday
- Join us for COMP industrial and academic mentor lunches during the meeting

COMP Newsletter

Statement from the Chair

Wendy Cornell, COMP Chair 2008, reports on the division's status

The COMP Division remains in good financial health and able to offer a well defined slate of quality benefits to our members. Programming at the national meetings continues as a centerpiece for the division and Program Chair Jeffry Madura has scheduled a number of interesting symposia for the Fall 2008 meeting in Philadelphia, PA. Awards Chair Carlos Simmerling oversaw the selection of winners of the CCG Student Excellence and HP Junior Faculty Awards and those scientists will be recognized at the Tuesday evening Poster Session.

Those of you who like to ski should take note that the Spring 2009 meeting will take place in Salt Lake City, UT, an exotic new locale for ACS. In Fall 2009 we return to Washington, D.C. Not everyone is able to attend the national meetings, but every member should receive Annual Reports in Computational Chemistry (ARCC). Editors David Spellmeyer and Ralph Wheeler are close to wrapping up another fine volume (4), due to ship later this year. The division took a carefully calculated financial risk when it launched this series a few years back and we are pleased that it has paid off and been well received by our members.

COMP elections are currently in progress and we thank Secretary John Woolfrey for setting up the electronic ballots. We hope you will consult the candidate profiles and take the time to vote. If you are interested in being considered as a candidate in next year's election, please contact Chair Elect Hanneke Jansen.

The Fall 2008 Philadelphia meeting will mark the fourth instance of the COMP mentor lunches, where junior researchers in the field, usually graduate students and postdocs, have the opportunity to meet with one or two senior researchers from either academics or industry and learn more about careers in that field. A frequent topic of discussion is the interview and candidate selection process. The lunches benefit candidates and employers alike. Candidates learn how to identify appropriate opportunities and present themselves in the best light. And employers are advantaged when candidates present their skills and interests clearly.

The mentor lunches are coordinated by COMP Alternate Councilor Rommie Amaro and supported in part by BioSolveIT. Rommie herself recently took part in a job search, culminating in a position as an assistant professor. She credits her academic colleagues on the COMP Executive Committee with providing useful advice and is pleased to be able to arrange for other junior researchers in the field to make similar connections.

Speaking of connections, one of the objectives of our COMP Strategic Plan is to help strengthen the community of computational chemists. Chair-elect Hanneke Jansen takes particular interest in this goal and is working with COMP web master Allen Richon and others to investigate social networking capabilities for our web site. www.acscomp.org

Allen joined us as webmaster earlier this year and has undertaken a major enhancement of the site. Links were tested and dead ones removed, but if you happen to find one that he missed, do not hesitate to contact him! We are eager to hear your feedback in general:

- Do you like the look and feel of the site?
- Can you find the information you are looking for?
- What else would you like to see?
- Career resources
- Teaching resources
- Webcasts of presentations at national meetings
- Focused discussion groups
- Are you interested in helping with the site?

When you visit the web site, one difference you may notice is the sponsor logos displayed on the home page. COMP has a number of loyal sponsors that provide support at every national meeting as well as other sponsors that provide support for particular symposia of interest. Other sponsorship opportunities are associated with awards, social events, and ARCC. Thanks are due to Assistant Secretary Ed Sherer for collecting the logos. If you would like to see your company logo displayed on the web site, contact Treasurer Curt Breneman to learn more about COMP sponsorship opportunities.

Sometimes the shoe is on the other foot and COMP itself serves as a sponsor. This is the case, for example, with certain regional meetings that include one or more sessions of COMP related programming. If you are involved with planning a regional meeting and would like to apply for financial support, contact COMP Local Section and Regional Meeting Coordinator Phil Bowen at jpbowen@uncg.edu.

Finally, I would like to acknowledge outgoing COMP Treasurer Curt Breneman for the contributions he has made to the division in this position over the past nine years. The Treasurer has responsibility for ensuring that an appropriate balance exists between assets and programs and also for filing the annual federal tax return. Moreover, Curt was instrumental in setting up the HP Junior Faculty Awards and has also been actively involved in coordinating the CCG Student Excellence Awards and the Schrodinger Emerging Technologies Symposium. Thank you, Curt!

I end with an invitation for you to send us your comments, questions, and suggestions. Contact information for officers can be found on the COMP web site. And members are always welcome to approach us at national meetings. We plan to add photos to the web site very soon, to make it easier to recognize us.

Wendy Cornell

COMP Elections

Vote in the 2008 Elections for the Officers of the COMP Division

The 2008 ASC COMP Division elections are taking place between August 8 – September 19. This election is your opportunity to influence the composition of the COMP Division's Executive Committee. The positions to be filled this year on the Executive Committee are Chair, Treasurer, and Councilor.

The Chair-Elect candidates and biographies are presented in alphabetical order:

Curt Breneman

Dr. Curt Breneman is a Professor of Chemistry and Chemical Biology at Rensselaer Polytechnic Institute (RPI) in Troy, NY. Prior to his arrival at RPI in July of 1989 as an Assistant Professor, Curt earned a Ph.D. in Chemistry at the University of California, Santa Barbara (1987), and completed post-doctoral work with Professor Kenneth Wiberg at Yale in computational chemistry. Curt was promoted to Associate Professor in 1995, and advanced to Full Professor in 2002. During his tenure at RPI, Curt worked in the areas of both computational chemistry and chem-informatics. In addition to numerous publications and presentations in these fields, Curt and his research group have authored and distributed a number of specialized programs for computing molecular property descriptors that are based on the properties of rapidly computed molecular electron densities. Curt and his group have active collaborations within RPI, and with members of the greater mathematics and chemical engineering communities on the design of chromatographic displacers, and with members of the decision sciences and engineering systems faculty at RPI as part of the NSF Project DDASSL (Drug Design And Semi-Supervised Learning - see: http://www.drugmining.com). More recently, Curt was named director of the NIH Roadmap "Rensselaer Exploratory Center for Cheminformatics Research" (RECCR, http://reccr.chem.rpi.edu), which has become institutionalized as an RPI Center of Excellence for the development and dissemination of predictive cheminformatics methods and computational chemistry software.

Curt has been deeply involved with the Division of Computers in Chemistry for nine years as Treasurer, having first occupied that position in 1999. During this time, in addition to disbursing meeting expense checks and preparing financial reports, Curt helped to found and administer two major award programs - the CCG Excellence Award (for graduate students) and the Hewlett-Packard Outstanding Junior Faculty Award (for tenure-track faculty). For many years, Curt has also organized and chaired the Emerging Technologies in Computational Chemistry Award Symposium (sponsored by Schrodinger) which takes place at each Fall ACS meeting.

Curt has organized and chaired many COMP symposia, and has given numerous talks. In addition to that, he has worked behind the scenes at each ACS meeting since 1999 to make sure that the poster session and awards presentations are set up correctly and go smoothly.

If elected Chair of the Division of Computers in Chemistry, Curt pledges to use the knowledge he gained as Treasurer to not only improve the quality of our programming at National ACS meetings, but to continue the fundamental work of my predecessors in adding value to COMP membership through benefits such as the Annual Reports in Computational Chemistry (ARCC). He also promises to be responsive to changes in our field and is committed to devising new web-based methods for listening to your suggestions and collecting your feedback.

William Swope

William Swope is a computational chemist in IBM's Research Division at the IBM Almaden Research Center, in San Jose, CA, where most recently he has been involved in the scientific aspects of

IBM's Blue Gene Supercomputer program, helping to define, carry out and analyze computer simulations of protein folding on IBM's internal Blue Gene computers.

Besides microsecond scale simulation studies of protein folding thermodynamics and kinetics, Bill's current interests include comprehensive assessments of force field quality and the development of novel methods for QM/MM studies of liquids and solvation phenomena. Specifically, the QM/MM studies can be used to benchmark the quality of force fields, and to provide important insight about how and when force fields can be improved.

Bill obtained his undergraduate degree (B.A., 1975) in chemistry and physics from Harvard University, his Ph.D. in quantum chemistry (1979) from the University of California, Berkeley, under the direction of Prof. H. F. Schaefer, and then performed postdoctoral work in statistical mechanics at Stanford University with Prof. Hans Andersen. At Stanford, Bill worked on the theory and simulation of liquids, including simulation studies of liquid structure, phase transitions, condensation and solvation, performing early simulations to compute hydration free energies. At IBM Bill works in close collaboration with many other academic and industrial labs in areas related to protein simulation, force field development, and other aspects of drug discovery and development.

Bill was chair of the 2004 Computational Chemistry Gordon Research Conference where he worked to stimulate greater interaction between academic and industrial computational chemists. He was also the guest editor in 2001 of two special issues on deep computing in the life sciences of the IBM Systems Journal and the IBM Journal of Research and Development, both refereed journals that describe innovations in science related to computation.

In terms of a statement of scientific philosophy, Bill feels that theory and simulation have the greatest impact when they are coupled to complementary experimental efforts. Also, new mechanisms need to be encouraged to produce more and better academic-industrial interactions in computational chemistry. Finally, we need to stimulate the development of a new generation of techniques that blend quantum and classical methods for an accurate description of chemistry when it happens in the liquid phase and can treat important thermal and dynamical effects.

If elected Chair, I would strive to continue the excellent work of the COMP division, and to stress in particular means to support professional career development, mentoring programs for young professionals, outreach into K-12, greater interaction among academic, national laboratory and industrial computational chemists, and greater access to computational skills and tools within our community.

Other Positions on the Ballot:

The candidate for the Treasurer position is:

- **Chris Harwell** of D. E. Shaw Research, LLC.

The candidates for Councilor positions are:

- **Charles H. Reynolds** of Johnson & Johnson Pharmaceutical R&D
- **Ed Sherer** of Merck & Co., Inc.
- **Ralph A. Wheeler** of the University of Oklahoma

Biographical sketches of our candidates can be found online at:
http://www.acscomp.org/Division/officers/biographies2008.html
If you are a regular or associate member and did not receive an invite directly from the COMP secretary, you should send a note to elections@acscomp.org. Please include your name and ACS membership number in your email. We will verify that you are on the official member list. Once your membership is confirmed, you will receive the official invite with link to vote"

We have a wonderful group of individuals who are volunteering their time and talents to promote all aspects of Computers in Chemistry. Please support their commitment to the Division and vote as soon as you receive your electronic ballot!

Symposia for Philadelphia ACS Meeting

Highlights for Philadelphia ACS Meeting

The Fall 2008 meeting in Philadelphia promises to be interesting, as a number of COMP symposium organizers have scheduled a variety of topics ranging from drug discovery to computational methodology.

- Computational Approaches for Fragment Screening (Diane Joseph-McCarthy)
- Pharmacology: The Forgotten Art of Drug Discovery (Tudor I. Oprea)
- Free Energy Simulation: From Academic Research to Industrial Application (Wei Yang, Alexey Lugovskoy)
- Challenges in Computational Chemistry (Anthony Nicholls, Ajay N. Jain)
- Emerging Technologies (Curt M. Breneman)
- Molecular Mechanics Force Field Development (Yong Duan, Ray Luo)
- Combining Computational Chemistry with Sequence-Based Bioinformatics for Structure-Function-Activity Relationships (Troy Wymore, Charles L Brooks III)
- Poster Session (Emilio X. Esposito)
- CCG Excellence Award (Carlos Simmerling)
- Hewlett-Packard Scholar Awards (Curt M. Breneman)

- Exploring Chemical Reactions on Multiple Time and Length Scales with QM/MM Methods (Shawn T. Brown, Jochen Blumberger, Teodoro Laino)
- Targeting Protein Kinases in Drug Design (Elizabeth Lunney, S. Frank Yan)
- Quantum Chemistry (Adrian Roitberg)
- Molecular Mechanics (Emilio X. Esposito)
- Drug Discovery (IracheVisiers)

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.

If you have any ideas or would like to organize a symposium for the Spring 2009 National American Chemical Society Meeting in Salt Lake City or Fall 2009 Meeting in Washington D.C. please contact Jeffry Madura at madura@duq.edu.

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.

Organize a COMP symposium

If you would like to organize a symposium for the upcoming Spring or Fall National ACS meetings please contact Jeffry Madura, Emilio Esposito, or Adrian Roitberg.

HP Outstanding Junior Faculty Award Program

Sponsored by Hewlett-Packard

Hewlett-Packard and the ACS Division of Computers in Chemistry (COMP) are pleased to present four HP Outstanding Junior Faculty Awards for outstanding tenure-track junior faculty at the Fall 2008 ACS National Meeting. The award provides $1,000 to each of the four faculty members.

The 2008 (Philadelphia) winners are:

Lillian T. Chong, University of Pittsburgh, "Atomistic simulations of a two-domain protein switch: Mechanically-induced unfolding of one domain by the other"

Pengyu Ren, University of Texas at Austin, "Development of polarizable force field for ions"

Ravi Radhakrishnan, University of Pennsylvania, "Dynamic coupling machinery in DNA polymerases"

Artem E. Masunov, University of Central Florida, "Comparison of sum over states (SOS) and coupled electronic oscillator (CEO) formalisms used for computational design of two-photon absorbing materials with time-dependent density functional theory"

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, a 2-page extended abstract of the work and a letter of departmental support should be sent to Carlos Simmerling at carlos.simmerling@gmail.com.

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 provide $1,150 for travel expenses to the Philadelphia meeting and provide a one-year software license of CCG's Molecular Operating Environment (MOE) for their academic groups (http://www.chemcomp.com/). Each awardee will present a poster at the Divison's Tuesday evening poster session.

The awardees, in alphabetical order, are:

- Satyender Goel: "Derivation and implementation of the pairwise spin-contamination correction and application to study potential energy curves for 3-D transition metal hydrides from BS-DFT," *University of Central Florida*
- Lucius E. Johnson: "Mechanism of electronic stabilization of the 3MR and divalent carbon of cyclopropenylidene by amino-substitution: Comparison of topology of the electron density and orbital analysis methods," *University of Louisville*
- In Suk Joung: "Determination of alkali and halide monovalent ion parameters for use in explicitly solvated biomolecular simulations," *University of Utah*

- Laveena Muley: "The binding affinity awarded for hydrophobic bonding in scoring functions needs to be context dependent," *The State University of New York, Buffalo*

- Somisetti V Sambasivarao: "Systematic development of OPLS-AA force field parameters for ionic liquid simulations," *Auburn University*

Applications for awards to attend the meeting in Salt Lake City, UT in March 2009 consist of a 2-page extended abstract, 2-page CV, 1-page personal statement, and a supporting letter from the student's advisor and are due to Carlos Simmerling, carlos.simmerling@gmail.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.

COMP Mentor Lunch

Join us for lunch at the Philadelphia ACS National Meeting

Starting with the National ACS Meeting in San Francisco, COMP has been offering the possibility for junior members to have lunch with senior researchers. The goal is to allow for networking in an open, relaxed setting and to promote discussions about possible career paths in academia and industry.

Please join us in Philly, where we will offer two such lunches:

The academic mentor lunch will be on Monday, August 18 at noon and will be hosted by Orlando Acevedo (Auburn) and Rommie Amaro (UC Irvine). Get academic application and interview tips just in time for the academic recruiting season!

The industrial lunch will take place on Tuesday, August 19 at noon and will be hosted by BioSolveIT and Novartis. Come network and get the inside scoop on what it's like to work in industry!

Sign up sheets and meeting locations will be posted outside the COMP symposia starting on Sunday. Please sign up or email ramaro@mccammon.ucsd.edu if you are interested in attending.

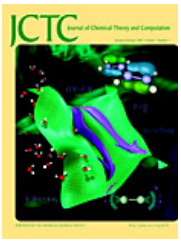
Journal of Molecular Graphics and Modelling

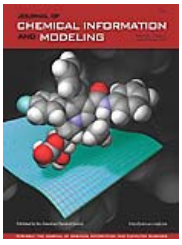
Submissions to JMGM are expanding rapidly, with over 300 manuscripts submitted in 2007! Elsevier published over 100 articles comprising 945 pages in that volume. JMGM now has twice as many pages allocated per year as it did when I became editor in 2000. Much of that is due to your excellent submissions and service as referees. Elsevier Science considers the Division's association with JMGM to be one of its most successful relationships. Keep the papers coming!

As always, thanks to you and the Editorial Board for your help and support.

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 second year of receiving an impact factor, *JCTC* ranked in the top 20 in Multidisciplinary Chemistry with an ISI Impact Factor of 4.308. It received 1,526 total citations in 2007.

In the category of Computer Science, Information Systems, *JCIM* ranks #2 in citations with 7,113 total cites out of 92 journals in that category. The journal received an ISI Impact Factor of 2.986.

Emerging Technologies Award

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

The COMP Division of the ACS will hold the eighth annual Symposium on Emerging Technologies in Computational Chemistry at the ACS National Meeting, Philadelphia, PA, on August 17. 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 an

extended (~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 meeting.

Thomas Kuhn Paradigm Shift Award

A stipend of $1000 and a platform to question the scientific status quo

The Thomas Kuhn Paradigm Shift Award is given each year to the talk that most captures the spirit of Kuhn's writings, exemplified in his landmark book, "The Structure of Scientific Revolutions". The symposium at each Spring ACS is open to all and attempts to attract those whose work has the potential to change the way we think about an aspect of science. Kuhn's words for this, a "Paradigm Shift", have been much over used and as such can be an intimidating standard to approach, but the intent is for talks that represent a fresh way of looking at an aspect of our field. As an example, the 2006 winner, Christopher Bayly of Merck-Frosst, proposed that focused screening was a more efficient path to drug discovery than high throughput screening. In 2008 Derek Debe of Abbott Laboratories presented the case for knowing confidence intervals in molecular modeling. Talks are generally sought from the computational sphere or fields with direct bearing upon it. They are judged on novelty, potential impact and quality of presentation by a panel of independent scientists with extensive computational experience. It is hoped the Award, which carries a stipend of one thousand dollars, can provide a platform for researchers extending a mirror to our field and questioning the scientific status quo.

Anthony Nicholls

236th National ACS COMP Sponsors

The COMP division would like to express gratitude to the following companies for their support of our programming at the 236th National ACS meeting.

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