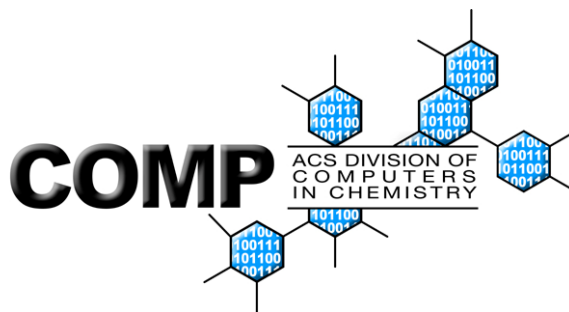


- J. Andrew McCammon to be Honored Tuesday Afternoon with the ACS Award for Computers in Chemical & Pharmaceutical Research
- William A. Goddard III is the winner of the 2008 ACS Award in Theoretical Chemistry
- Division's CCG Excellence Awards and HP Outstanding Junior Faculty Awards to be presented on Tuesday Evening



COMP Newsletter

Statement from the Chair

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

Most people I interact with through COMP know little about how the division functions. For starters, the Chair position, which I currently hold, is distinct from the Program Chair position, which I held from 2002-2004 and has henceforth been occupied by Jeffrey Madura. The Program Chair is an appointed position responsible for identifying symposium topics and organizers for the national meetings and for making the overall program come together within the OASYS system. This is no small feat. Sessions must be spread evenly across the week. Everyone wants to be scheduled on Sunday or Monday. And perhaps worst of all, sometimes the coffee and donuts do not show up. Nevertheless, based on your feedback, programming is something the division has done very well in recent years and we are proud of that.

The Chair, on the other hand, serves as chief executive on the Executive Committee and ensures that the business of the division gets accomplished according to ACS and division bylaws. Chair is an elected three-year position, beginning with a year as Chair Elect, a year as Chair, and a final year as Past Chair. I mention all of this so that you will better understand how we operate and also to introduce the notion

that I had a contemplative past year as Chair Elect in which I could consider what we as a division do well and what we could do better.

In my opinion, the following are examples of "what" we do well -

- Programming at national meetings
- Career Awards (CCG Student Excellence and HP Outstanding Junior Faculty)
- Symposium Awards (Emerging Technologies and Thomas Kuhn Paradigm Shift)
- Informational Career Support (Student Mentor Lunches and Career Symposia)
- Published content ("Annual Reports in Computational Chemistry")

and the following are examples of "how" we do well, through -

- Flexibility
- Inclusiveness and diversity
- Strategic planning

Areas where we could do better include -

- Operational efficiency
- Communication with members and potential members

Immediate Past Chair Ralph Wheeler initiated efforts to increase our operational efficiency by proposing the creation of two new positions – Assistant Secretary and Assistant Treasurer – as well as an Awards Committee. I am pleased that this January Ed Sherer and Chris Harwell joined the Executive Committee as Assistant Secretary and Assistant Treasurer, respectively. When Ralph solicited nominations for Assistant Treasurer I immediately thought of Chris, whom I had worked with in my previous job, and whom I knew was extremely responsible and effective at making sure the bills were paid! Ed, although a more recent acquaintance, came highly recommended for his organizational skills and service orientation. We welcome both onboard and are glad they will be able to support new Secretary John Woolfrey and long serving Treasurer Curt Breneman in their duties.

For Awards Committee Chair, we recruited Carlos Simmerling, a COMP Councilor whose students number among past winners of the CCG Award and who remembers what it was like to be a junior faculty member looking for financial support and scientific recognition. Carlos has taken responsibility for soliciting applications and judges for the CCG Student Excellence, HP Outstanding Junior Faculty, Schrodinger Emerging

Technologies, and OpenEye Thomas Kuhn Paradigm Shift Awards.

The communication challenge has been partly one of our own making. We simply did not want to spam our members with potentially unwanted e-mail. In recent years we have been using CCL to disseminate information about awards, symposia, etc, but this only reaches a fraction of the membership. We have therefore decided to experiment with a change in policy and e-mail members twice a year with the newsletter. We also decided to undertake a redesign of the web site and this January longtime COMP member and career symposium speaker Allen Richon came onboard as webmaster. The new website can be found in a new location – www.acscomp.org. We hope you will give us feedback on both initiatives.

With additions to the Executive Committee also come departures. In 2008 we bid farewell to two longtime members who have distinguished themselves by their service both inside and outside of COMP. Lisa Balbes served the division as web maven from 2000 through 2007 and was instrumental in launching the first electronic election for COMP, with substantial cost savings to the division. Lisa has also been active as a Career Consultant with ACS and was quoted in a December 11, 2007 article in the New York Times entitled “As Drug Industry Struggles, Chemists Face Layoff Wave.” Michelle Franci served the division as Secretary, Councilor, and Chair and launched our Flashmob Supercomputing events. Michelle is a gifted communicator whose podcasts on quantum chemistry are available on iTunes. Lisa and Michelle, we wish you the best and look forward to reading more about your accomplishments.

Wendy Cornell

Statement from the Past Chair

It seems like just yesterday that I was beginning my term as the COMP Division's new Chair and coordinating our long-range strategic planning session with your leaders and with professional facilitators from the ACS. That session

resulted in a Strategic Plan for the COMP Division to lead the innovative use of computers in experimental, theoretical and computational chemistry. The Executive Committee's primary 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. Thus, 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 strategic 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 achieve these goals during the past year, the COMP Division started several new initiatives and continued other successful projects: (1) a program of mentoring lunches was initiated, coordinated by Drs. Wendy Cornell and Rommie Amaro, (2) robust scientific and technical programming continued at national meetings under the able leadership of the Program Chair, Professor Jeffry Madura, (3) unprecedented member access was provided to some of the world's uniquely valuable computational chemistry literature, including Volume 3 of *Annual Reviews in Computational Chemistry* (ARCC), co-edited by Drs. David Spellmeyer and Ralph Wheeler, (4) the Executive Committee voted to contract with Dr. Allen Richon to renovate and maintain the Division's website and (5) nominations were solicited for the new appointed positions of Assistant Treasurer and Assistant Secretary to distribute the increasing workload brought about by the increasing number of Divisional projects.

Last year was a busy year for me as Chair and I want to thank all the COMP

Division's leaders for investing their time, energy, and creativity to help the COMP Division reach its strategic goals. Without their efforts, the Division could not function. My special, personal thanks go to our 2007 Secretary, Dr. Hanneke Jansen, and Treasurer, Prof. Curt Breneman, whose knowledge, skills, and help were invaluable to me. Special thanks also go to Lisa Balbes, for a job well done over many years as the Division's Webmaven. We wish you well, Lisa, in your expanding ACS duties. Finally, as I leave the Chair's position in the hands of Dr. Wendy Cornell (who is already well on her way to being a truly outstanding Chair), I thank the COMP members for giving me the opportunity to serve you as Division Chair and to work with the wonderful, dedicated individuals who are the Division's leaders!

Ralph A. Wheeler

Symposia for New Orleans ACS Meeting

Highlights for New Orleans and preview of the Philadelphia ACS Meeting

The Spring 2008 meeting in New Orleans 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 American Chemical Society Meeting in New Orleans will feature 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 Salt Lake City meeting (Spring 2009) 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)

The poster session will take place as usual on Tuesday night. The CCG Student Excellence Award and the Hewlett-Packard 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.

A number of symposia are in place for the Fall 2008 meeting in Philadelphia. Symposia:

- Challenges in Computational Chemistry (Anthony Nicholls, Ajay N. Jain)
- Combining Computational Chemistry with Sequence-Based Bioinformatics for Structure-Function-Activity Relationships (Troy Wymore, Charles L Brooks III)
- Computational Approaches for Fragment Screening (Diane Joseph-McCarthy)
- Drug Discovery (Irache Visiers)
- Emerging Technologies (Curt M. Breneman)
- Exploring Chemical Reactions on Multiple Time and Length Scales with QM/MM Methods (Axel Kohlmeyer)
- Free Energy Simulation: From Academic Research to Industrial

Application (Wei Yang, Alexey Lugovskoy)

- Poster Session
- CCG Excellence Award (Andrew Good)
- Hewlett-Packard Scholar Awards (Curt M. Breneman)
- Molecular Mechanics Force Field Development (Yong Duan, Ray Luo)
- Pharmacology: The Forgotten Art of Drug Discovery (Tudor I. Oprea)
- Targeting Protein Kinases in Drug Design (Elizabeth Lunney, S. Frank Yan)
- General Oral – Quantum Chemistry (Adrian Roitberg)
- General Oral – Molecular Mechanics (Emilio X. Esposito)
- General Oral – Drug Discovery (Irache Visiers)

ACS Award for Computers in Chemical & Pharmaceutical Research

Sponsored by Schrödinger

SCHRÖDINGER

Professor J. Andrew McCammon of University of California, San Diego is the winner of the 2008 ACS Award for Computers in Chemical and Pharmaceutical Research for his contributions to the fields of protein modeling and computational drug design.

Dr. McCammon received his A.B degree at Pomona College and his Ph.D. degree in chemical physics from Harvard University. After two years as a research fellow at Harvard, McCammon joined the faculty at the University of Houston for 16 years until he moved in 1994 to his current appointment as the Joseph E. Mayer Chair of Theoretical Chemistry at UC San Diego.

Professor McCammon will present his award address “Adventures in computational chemistry” before the COMP Division on Tuesday afternoon. This award is generously sponsored by Schrödinger.

ACS Award in Theoretical Chemistry

Sponsored by IBM Corp.

IBM

Professor William A. Goddard III of CalTech is the winner of the 2008 ACS Award in Theoretical Chemistry. His work has laid the foundation for GVB theory and has advanced the knowledge of quantum chemistry.

Dr. Goddard received his B.S. degree at the University of California, Los Angeles and his Ph.D. degree in engineering from CalTech. Goddard joined the faculty at CalTech in 1965 and has remained there his entire career.

Professor Goddard will present his award address before the Division of Physical Chemistry.

HP Outstanding Junior Faculty Award Program

Sponsored by Hewlett-Packard

hp
i n v e n t

Hewlett-Packard and the ACS Division of Computers in Chemistry (COMP) are pleased to present five HP Outstanding Junior Faculty Awards that provide \$1,000 in travel funds, a special gift from Hewlett-Packard, and recognition at the COMP poster session awards ceremony in New Orleans to each of the five outstanding tenure-track junior faculty selected.

The 2008 winners were:

Micah L. Abrams, "Determination of absolute configuration in solution", University of Central Arkansas, Conway, AR

Orlando Acevedo, "Advances in potentials of mean force methodology for organic and biological simulations", Auburn University, Auburn, AL

So Hirata, "Predictive electronic and vibrational many-body methods", University of Florida, Gainesville, FL

Shuxing (King) Zhang, "Integration of a bioinformatics approach to high-throughput docking and its application to the discovery of novel TNF receptor-associated factor 6 (TRAF6) inhibitors", MD Anderson Cancer Center, Houston, TX

Wei Yang, "Problem Oriented Sampling Design Towards Quantitative Biomolecular Simulations" Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL

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. Postdoctoral researchers in transition to faculty appointments may also be considered. Selection criteria will include the novelty and importance of the work to be presented, as well as the level of Departmental support as indicated by a letter of support by the Chair or Chair designee.

To apply for an award for the 237th ACS National Meeting in Salt Lake City, UT, March 22-26, 2008, an extended abstract of the work (no more than 2 pages) and the letter of departmental support should be sent to **Carlos Simmerling** at: carlos.simmerling@gmail.com.

Chemical Computing Group Excellence Awards 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 New Orleans meeting and one-year software license for the CCG Molecular Operating Environment (MOE). (<http://www.chemcomp.com/>)

The awardees, in alphabetical order, are:

- Hanning Chen, University of Utah, "Hydrophobic Interaction in Acidic Aqueous Solutions"
- Pablo Englebienne, McGill University, "FORECASTER: A new platform for drug discovery"
- Jeff Hammond, Pacific Northwest National Laboratory, "Coupled-cluster theory on supercomputers"
- Sapna Sarupria, Rensselaer Polytechnic Institute, "Using computer simulations to explore pressure effects on proteins"
- Jean-François Truchon, Université de Montreal, "Considering a treatment of induced electronic polarization based on the Poisson equation"

Applications for awards consist of an extended abstract, CV, personal statement, and a supporting letter from the student's advisor and are due to **Carlos Simmerling** at carlos.simmerling@gmail.com. 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

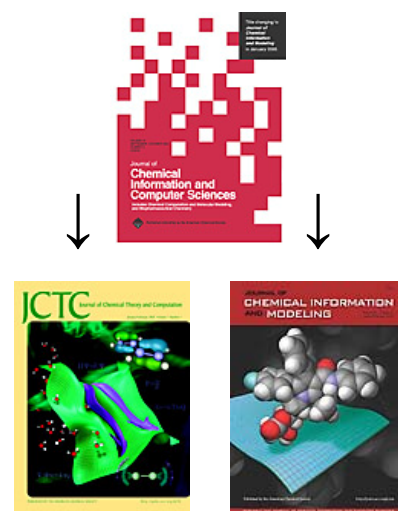
online submissions prior to the deadline for the meeting at which the awards will be presented. Submissions are restricted to North, Central and South American students. Please see the COMP website for more details.

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

How JCICS led to JCTC and JCIM



The *Journal of Chemical Information and Computer Sciences (JCICS)*, under the editorship of Bill Milne, flourished during the period 1975-2004. From its roots in chemical information and library science, the journal evolved to publish papers in many areas of computational chemistry including molecular modeling, graph theory, database searching, computer-aided molecular design, and QSAR.

In 2003, *JCICS* was monitored by the Joint Board Council Committee on Publications

(JBCCP) as part of its routine duties of oversight. At the same time, a new Editor was sought for the journal. A JBCCP subcommittee was appointed to formulate options for consideration. It was decided that *JCICS* was serving two audiences: (1) information science, molecular modeling, database searching, cheminformatics, pharmaceutical applications of computational chemistry, and (2) computational quantum chemistry. An Editor was identified who could bridge these two areas, Bill Jorgensen (Yale University), and he was keen to split the portfolio into two parts. *Journal of Chemical Information and Modeling (JCIM)* and *Journal of Chemical Theory and Computation (JCTC)* began publication in January 2005. *JCIM* publishes, "Papers reporting new methodology or important applications in the fields of chemical informatics or molecular modeling..." *JCTC* publishes papers reporting new theories, methodology, or important applications in quantum chemistry, molecular dynamics, and statistical mechanics.

Peter Jurs

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>.

COMP website continuously improving

The COMP website has updated its look.

The COMP website will continue to be improved under our new website administrator, Allen Richon. The website currently features new information and awards related to the COMP division and its members. In addition, two employment RSS related feeds are available. 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://www.acscomp.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*

How can COMP reach you?

Updating your contact information.

Communications and benefits from the COMP Division to its members sometimes disappear in a void due to incorrect or outdated addresses. Items of importance and value include the COMP elections and the *Annual Reports in Computational Chemistry (ARCC)*. The elections have been held electronically over the past 2 years and require a valid email address on file with the ACS. The ARCC mailing requires a valid street address that has not been flagged as a "bad address" on the ACS roster. The latter happens when mailings have been returned to sender in the past. We encourage all our members to check the validity of email address and street address in their ACS profile, especially existing members who have not received the electronic election invites or the ARCC mailings.

You can check and change your address(es) on-line by logging in to the ACS home page and going to "edit my profile". You can also contact ACS Customer Service (1-800 333-9511 US or 614-447-3776 outside of US). The representatives from this department will

be able to visually confirm whether your address has a "bad address" flag present.

Join the COMP division!

<http://www.acscomp.org>

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

Newsletter Correction/Addition

In the original Spring 2008 COMP newsletter, sponsorship of the 2008 ACS Award for Computers in Chemical and Pharmaceutical Research was incorrectly attributed to Accelrys Inc. This updated version gives the appropriate credit to Schrödinger. We apologize for the error.

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