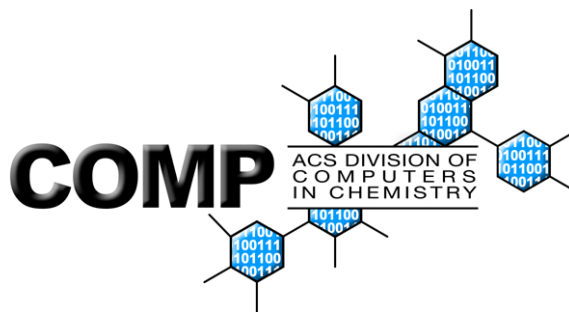


- 6 COMP members selected as ACS Fellows
- Division's CCG Student Excellence Awards and HP Outstanding Junior Faculty Awards will be Presented On Tuesday
- "Leaving the Nest: Life after Post-Doc'ing" event on Monday from 5-7 pm



COMP Newsletter

Statement from the Chair

*Hanneke Jansen, COMP Chair 2009,
reports on the division's status*

In clicking through my archives to remind myself of all the COMP-related activities since my previous contribution to the Spring Newsletter, I am amazed and grateful. Amazed at how many things have happened and grateful for the work of the many volunteer leaders of the Division and the Society.

The Division's website has undergone a facelift, courtesy of Allen Richon, our Webmaster. If you haven't visited in a while, I encourage you to check it out at www.acscomp.org. If you have content that you would like to share or see presented on the website, please contact us. Contact information for all elected and appointed division leaders is available on our website and at the end of this newsletter. We have also posted pictures of many of us there so you can recognize us when you attend COMP-related events.

In addition to the website, the Division has an online presence on LinkedIn and Facebook. I encourage you to join those groups to connect with likeminded people, share news, ask questions and discuss. Patrick Lee has taken responsibility to set up these COMP communities and post executive committee business there. We rely on all of you, our members, to

contribute to these sites in order to make them useful and interesting, which will help build and nurture our community.

The COMP together initiative, which I briefly mentioned in the Spring Newsletter, is continuing and we are getting ready to start pilot events. This initiative includes tools and a network of local "champions" to facilitate COMP members getting together on a local and informal level (seminars, networking events, mentoring lunches). We will send out notifications about who the local champions are for the various areas for which we have coverage. If your area is not covered, we'll try to work with you to identify local champions and figure out whether there are enough COMP-minded people in that geographical area to start hosting events with. If you are in an area where there isn't a sufficient presence, we again encourage use of the LinkedIn and Facebook groups.

A new American Chemical Society (ACS) initiative that was launched this year is the ACS Fellows Program. This Program has as its overarching goal "to recognize members of the American Chemical Society for outstanding achievements in and contributions to science, the profession, and the society." Nominations for ACS Fellows were sought from divisions, local sections, committees, and individuals. We decided that the COMP divisional

nominations would be coordinated by the Chair succession (Chair-elect, Chair, and immediate past-Chair). The three of us gathered input from the divisional leadership, selected several high quality candidates, solicited and wrote nomination letters and put together and submitted the nomination packages. You will see a listing of all COMP members who were selected as ACS Fellows in this Newsletter (this includes divisional as well as other nominees). I want to thank my colleagues in the Chair succession and all the secondary nominators we worked with for their efforts to make sure COMP has an excellent presence in this first class of ACS Fellows. A final note on this topic is that divisional nominations can only be made for members of the nominating division and all nominators (primary and secondary) must be division members as well. This highlights a new COMP membership benefit: you can be a divisional secondary nominator or a divisional nominee for ACS Fellow.

The COMP symposia at the national meetings continue to be prime events for dissemination of top quality scientific content and for meeting and discussing with fellow scientists. Program Chair Jeffry Madura and Assistant Program Chairs Emilio Esposito and Adrian Roitberg have assembled another outstanding program for the upcoming Fall meeting in Washington

DC. I hope to see many of you at the various symposia they coordinated and put together.

Students and post-docs are particularly invited to the "Leaving the Nest: Life after Post-Doc'ing" symposium, scheduled for Monday August 17th and organized by Lisa Balbes. This session will introduce ideas of interest to computational chemistry graduate students and post-docs who are thinking about their next job. A panel of 5 scientists with different employment histories will provide words of wisdom from their personal experience, and will mix informally with attendees during a pizza dinner in the latter part of the session. Rommie Amaro continues to organize mentor lunches on behalf of the COMP Division, also aimed at graduate students and post-docs (see announcements of these events in this Newsletter).

The COMP Division's commitment to dissemination of top quality scientific content extends beyond the programming at the national meetings and includes our publication of the *Annual Reports in Computational Chemistry*, ARCC. Volume 5 in this series is in the making and thanks go to the editor, Ralph Wheeler, and all his section editors and authors for another excellent volume. All COMP members on the 2008 year-end list will receive this book in a couple of months. If resources permit, we will include members who joined during 2009 with the note that their join-date determines their rank on the list of those possibly included in the mailing.

The Division held its annual elections over the summer and the outcome is published in this Newsletter. Here, I want to specifically thank Assistant Secretary Ed Sherer for running a very smooth election which resulted in an increased participation of our membership. In addition to elections, we involve volunteer leaders through appointed positions to deal with specific needs of the division. The executive committee is working on appointing a new Assistant Treasurer to assist in streamlining the divisional administration as well as expanding the work we do in support of the Division's mission. We are looking at ways to more efficiently connect with our sponsors and do fundraising. We are very

grateful for our many sponsors who have been, and are, supportive of the Division. Some of the sponsors have had to cut back because of the current economic situation and the Division will have to find ways to manage this. If your company is in a position to sponsor an event, an award or a symposium, I encourage you to contact our Treasurer, Chris Harwell. The Division also decided to bring the role of Coordinator of Local Section/Divisional Activities into the portfolio of Treasurer and Assistant Treasurer. We thank Phil Bowden for his years of service in this role. Finally, the appointment of an Assistant Treasurer will also give us an opportunity to support the COMP together initiative which may result in sponsorship for local events that will have to be managed.

In closing, I want to highlight an exceptional COMP leader who has contributed tremendously to the division and our scientific discipline: Wendy Cornell. Her term as an elected member of the executive committee is coming to an end and I want to thank her, both personally and on behalf of the rest of the division's leadership, for all she has contributed. Wendy was involved in programming for the national meetings from 2001-2006, first as Assistant Program Chair and then as Program Chair. She was subsequently elected as Chair of the Division, serving as Chair-elect in 2007, Chair in 2008 and immediate past Chair in 2009. During her tenure as Chair she focused especially on increasing operational efficiency and communication with (potential) members. Those are still critical elements of our work today. Wendy, we hope to be able to call on you in the future for guidance and inspiration!

The above are highlights of the many things your divisional leadership is working on and the names of some of the volunteer leaders. We welcome your ideas and suggestions, as well as your time and energy as a volunteer, for new initiatives or improvements to some of the things we are currently working on.

Hanneke Jansen

ACS Fellows (COMP members)

The COMP Division congratulates the six members of our Division who have been selected for the first (2009) class of ACS Fellows. These members share a common set of accomplishments, namely true excellence in their contributions to the chemical enterprise coupled with distinctive service to ACS or to the broader world of chemistry. We thank them for their commitment and service.

The awardees, in alphabetical order, are:

Michelle M. Francl
Bryn Mawr College

Kendall N. Houk
University of California, Los Angeles

William L. Jorgensen
Yale University

Peter C. Jurs
Pennsylvania State University

David C. Spellmeyer
Nodality

Gregory A. Voth
University of Utah

2009 COMP Election Results

COMP Division Election News

We are excited to announce the results of the 2009 COMP elections:

The 2010 chair-elect of the COMP division is Kate Holloway. Dr. Holloway received her Ph.D. from the University of Texas at Austin and is now a Senior Research Investigator at Merck.

Carlos Simmerling and Peter Jurs were elected councilors for the 2010-2012 term. Dr. Simmerling is Professor of Chemistry at Stony Brook University and Dr. Jurs is Professor Emeritus of Chemistry at Pennsylvania State University.

The two elected alternate councilors for the 2010-2012 term are Adrian Roitberg and Rommie Amaro. Dr. Roitberg is an associate professor of chemistry at the University of Florida and Dr. Amaro is an assistant professor at University of California, Irvine.

The executive committee of the COMP division would like to thank all the candidates for their willingness to run and serve the Division's membership. We also gratefully acknowledge the other candidates for office, Luke Achenie and Bill Swope. Luke will remain active as COMP's MPPG representative. We would also like to thank Ed Sherer for running the elections smoothly and on time and to Curt Breneman and Jeffrey Madura for help with the nominations.

We look forward to what our new elected officers will bring to the COMP division!

Melissa Landon

Symposia for Washington D.C. ACS Meeting

Highlights for Washington D.C. ACS Meeting

The Fall 2009 meeting in Washington D.C. promises to be interesting, as a number of COMP symposium organizers have scheduled a variety of topics ranging from drug discovery to computational methodology.

- The Role of Quantum Chemistry in Chemical Biology and Medicinal Chemistry (Antonio M. Ferreira)
- Structure Activity Relationship Knowledgebases (Evan Bolton, Stefan Senger)
- Protein Dynamics and Function (Huan-Xiang Zhou, Gerhard Hummer)
- Computational Chemistry in the Discovery & Development of Novel Anti-Infective Agents (G. Scott Weston, Ryszard J. Czerminski, John I. Manchester)

- Simulation of (Bio)Organic-Inorganic Interfaces and Nanostructures Using MD, MC, and Multiscale Approaches (Hendrik Heinz)
- Scripting and Programming (Joseph M Leonard, Jeff R. Hammond, Chris Harwell, Rommie E Amaro, Rajarshi Guha)
- Emerging Technologies (Curt M. Breneman)
- Leaving the Nest: Life After Post-Doc'ing (Lisa M Balbes, Jeffrey D. Madura, Emilio Xavier Esposito)
- Molecular Visualization (Rommie E Amaro, Emilio Xavier Esposito)
- Poster Session (Emilio X. Esposito)
- CCG Excellence Award (Carlos Simmerling)
- Hewlett-Packard Scholar Awards (Curt M. Breneman)
- Quantum Chemistry (Adrian Roitberg)
- Molecular Mechanics (Emilio X. Esposito)
- Drug Discovery (Irache Visiers)

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 2010 National American Chemical Society Meeting in San Francisco or Fall 2010 Meeting in Boston please contact Jeffrey 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 Jeffrey 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 2009 ACS National Meeting. The award provides \$1,000 to each of the four faculty members.

The 2009 (Washington D.C.) winners are:

Donald Hamelberg, Georgia State University, "Accelerated molecular dynamics in studying long-timescale biomolecular events"

David L Mobley, University of New Orleans, "Computational predictions of binding affinities"

Jose A. Gascon, University of Connecticut, "Integrating electronic-embedding QM/MM approaches with implicit electrostatic solvent models"

Chia-en A. Chang, University of California at Riverside, "Multiscale simulation methods for protein dynamics and synergistic regulation of enzyme complexes"

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, a CV, and a letter of departmental support should be sent to Carlos Simmerling,

(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 Washington D.C. 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 Division's Tuesday evening poster session.

The awardees, in alphabetical order, are:

- **Sourav Das**: "Pair-wise property-encoded shape distribution descriptors applied to prediction of

protein-ligand binding affinities," *Rensselaer Polytechnic Institute*

- **Fangyu Ding**: "Drug pressure induced mutations in HIV-1 protease alter flap conformations," *Stony Brook University*
- **James I. Fells Sr.**: "Binary QSAR study for identifying selective LPA₃ antagonists," *University of Memphis*
- **Kiumars Shahrokh**: "Quantum mechanics-coupled AMBER ff99 compatible heme parameters for the P450 catalytic cycle," *University of Utah*
- **Lai Xu**: "Dynamics of 1,3-dipolar cycloadditions of diazonium betaines to acetylene and ethylene: Bending vibrations facilitate reaction," *University of California, Los Angeles*

Applications for awards to attend the meeting in San Francisco, CA 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 Lunches

Join us for lunch at the Washington D.C. ACS National Meeting

Starting with the 232nd 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 Washington D.C. on Tuesday, August 18 where we will offer a mentor lunch at noon.

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

Sponsored by:



Journal of Molecular Graphics and Modelling

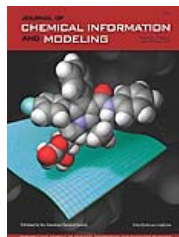


The *Journal of Molecular Graphics and Modelling (JMGM)* is devoted to the publication of papers on the uses of computers in theoretical investigations of molecular structure, function, interaction, and design. The scope of the journal includes all aspects of molecular modeling and computational chemistry, including, for instance, the study of molecular shape and properties, molecular simulations, protein and polymer engineering, drug design, materials design, structure-activity and structure-property relationships, database mining, and compound library design.

JMGM is co-edited by Jeffrey D. Madura at Duquesne University and J. D. Hirst at University of Nottingham. The journal received an ISI Impact Factor of 2.347 in 2008.

Comp members are encouraged to use JMGM, JCTC, and JCIM (see below) as a forum for their publications. Articles describing research of substantial merit are invited.

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. JCTC is also co-edited by Gustavo E. Scuseria at Rice University.

JCTC ranks in the top 20 in Multidisciplinary Chemistry with an ISI Impact Factor of 4.274. It received 2,525 total citations in 2008. ScienceWatch.com recently featured the journal for June 2009, and Thomson Reuters named JCTC as a rising star in the field of Chemistry.

In the category of Computer Science, Information Systems, JCIM ranks #2 in citations with 8,444 total cites out of 99 journals in that category. The journal received an ISI Impact Factor of 3.643.

Nanoscience Presentations Online

The theme for the ACS Spring National Meeting in Salt Lake City was Nanoscience: Challenges for the Future, organized by Professor Paul Weiss, Pennsylvania State University and Editor-in-Chief, ACS Nano.

By many accounts, the thematic program was a great success with 20 technical divisions making significant contributions to the nanoscience program. COMP was an

“Leaving the nest: Life after post-doc’ing” Monday evening, 5-7PM, 147B Convention Center

Join COMP for a panel discussion and networking session to help provide you with the knowledge and tools you need to make your next career move in the right direction. We will discuss:

- Different types of employers - academic, industrial and government, their subtypes and expectations
- How to find employment in each field
- Resumes, curriculum vitae (CV), and the other documents that should make up your employment portfolio.
- Nontechnical skills and knowledge crucial for continual career development
- Career ladders and nontraditional career fields

active part of the Salt Lake City nanoscience program.

During the meeting select sessions were recorded within the nanoscience program including the Keynote Address and the Plenary Session. Those presenters who gave us permission to record their presentations are located at <http://www.softconference.com/ACSchem/>. Please have a look and let us know what you think about this new offering by the ACS.

For additional information on this activity, please see the [March 16 ACS Comment Column in C&EN](#) (Vol. 87, No. 11, p. 62) by Kent Vorhees, ACS Director-at-Large, which discusses using this new technology to expand access to ACS national meeting content.

Richard Love

COMP and CCL

The COMP division is a proud sponsor of the Computational Chemistry List (CCL) at <http://www.ccl.net>.

Please check the CCL for information regarding upcoming COMP events, awards, and news.

238th National ACS COMP Sponsors

The COMP division would like to express gratitude to the following companies for their support of our programming at the 238th National ACS meeting.



How can COMP reach you?

Updating your contact information.

You can check and change your email and mailing addresses 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.

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