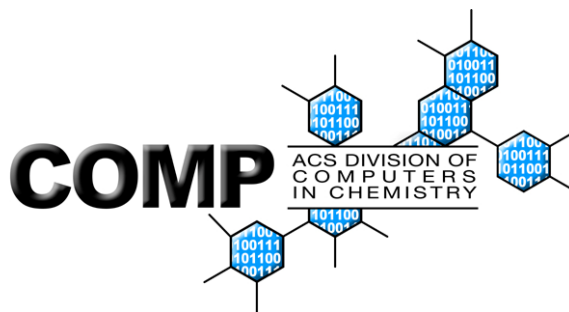


- COMP wins a 2010 ChemLuminary Award
- Division's CCG Student Excellence Awards and HP Outstanding Junior Faculty Awards will be Presented on Tuesday Evening
- Mentor Lunch on Tuesday at Noon



COMP Newsletter

Statement from the Chair

M. Katharine Holloway, COMP Chair 2011, reports on the division's status

As 2011 Chair of COMP, I'd like to welcome you as a new or continuing member of the division!

During my year as Chair-elect in 2010, I've been getting to know you. So, who is COMP? As it turns out, we are comprised of over 2200 scientists. About half are academics and half are in government or industry. While about a quarter have more than 10 years of service, another quarter are students just beginning their careers. Of those reporting their citizenship, there are almost 50 countries represented! And our research spans the gamut from molecular mechanics to molecular dynamics to quantum mechanics, from drug discovery to materials research, from gas-phase to solvated systems, from cheminformatics to new computational methods. In order to provide value to such a diverse population, we have some pretty diverse member benefits.

For those of you attending one or both of the national meetings, we have a full schedule planned for you this year. At the spring meeting in Anaheim, there will be 52 invited talks, 145 contributed talks, and 127 posters presented in 49 half-day sessions. Be sure to check out the image on the cover of our program brochure. It

was selected as the winner of our first image contest.

If you can't make it to the Anaheim meeting, 3 of our sponsored or co-sponsored symposia were chosen to be recorded and made available on the ACS web site after the meeting:

- ACS Award for Computers in Chemical and Pharmaceutical Research symposium in honor of Thom Dunning
- Docking & Scoring: A Review of Docking Programs
- Pioneers of Quantum Chemistry (co-sponsored with HIST)

We also anticipate a great program at the fall meeting in Denver. As a reminder, abstracts are due Monday, April 4th, 2011. Many thanks to our program chair, Emilio Esposito, and members of our program committee for a terrific job.

For those who won't be attending a national meeting this year, COMP Together, our new local networking initiative, might be just what you're looking for. It's intended to facilitate COMP members getting together informally at the local level for seminars, networking events, and mentoring lunches. You can register for COMP Together in your area at:

http://www.acscomp.org/COMP_Together/reg_form.php. In addition to participation,

we are seeking additional local champions who would be willing to organize events, coordinate presenters, scout for venues, and possibly engage sponsors. If you are interested in learning more about becoming a local champion, please indicate this when you register.

We also offer a regular peek at what's new in our field via the *Annual Reports in Computational Chemistry*, edited by Ralph Wheeler and David Spellmeyer. The 2010 volume included chapters on the use of GPUs for MD simulations, QM/MM methods in free energy simulations, developing antibiotics that target the ribosome, the folding of conjugated proteins, and protein-ligand scoring using Mean-Force or DFT approaches.

In addition, the COMP division awards committee, ably chaired by Carlos Simmerling, presents several awards each year to students (Chemical Computing Group Excellence Award and the Peter Kollman Graduate Award in Supercomputing sponsored by the National Institute of Computational Sciences); to young faculty (Hewlett-Packard Outstanding Junior Faculty Award); and to developers of novel methodology (Emerging Technologies in Computational Chemistry). The COMP division also holds a symposium to honor the winner of the ACS Award for Computers in Chemical

and Pharmaceutical Research sponsored by Accelrys. This year's awardee is Thom Dunning, whose *ab initio* basis sets are employed by many.

We also offer you the opportunity to become more involved in the ACS. All of our officers and representatives are volunteers. If you'd like to learn more, please contact me or one of the other COMP officers.

In closing, I'd like to congratulate the COMP division members who were named ACS Fellows in 2010 to honor their involvement with the ACS, as well as their commitment to science: Wendy Cornell (Merck), Chris Cramer (University of Minnesota), Kennie Merz (University of Florida), Chuck Reynolds (Ansaris), and Ralph Wheeler (Duquesne). Congratulations also to our new officers: Jeffry Madura (Chair-elect), Ed Sherer (Secretary), and Emilio Esposito (Councilor). And a special thanks to our other volunteers and to our financial sponsors.

Why don't you join us in getting involved with the COMP division, either at the national or local level? Whether you are a long-time member or have just joined the division, I look forward to getting to know you better this year.

Kate Holloway

COMP Mentor Lunch

Please join us in Anaheim, where we will offer an academic mentor lunch and an industrial mentor lunch on Tuesday, March 29 at noon. Groups will meet outside the COMP symposia and then depart for lunch at a local restaurant. Look for the signup sheets outside of the COMP symposia.

Lunches are limited to the first 10 people who sign up.

COMP wins 2010 ChemLuminary Award



Your COMP Division was awarded the coveted 2010 Divisional ChemLuminary Award for "Recognition of Innovation and Outstanding Service to Members of a Division" at the National Meeting in Boston! The award is very prestigious - a recognition by the ACS for the most active and innovative Division of the year.

The lead activity of the Division, co-sponsored with the Auburn Local ACS Section, was an innovative on-site workshop that involved the assembly of an "Instant Supercomputer" at the recent 2009 ACS Southeastern Regional Meeting (SERMACS) held in Puerto Rico. The workshop was entitled "Connecting Resources, Connecting Others: Supercomputing in the Global Age" and featured an interactive ad hoc cluster building demonstration. In keeping with the 2009 SERMACS theme "Think Positive, Think Global, Think Chemistry" COMP's goal was to underscore the importance of the cooperative spirit of science in a global age using the connection of solitary laptops to form a supercomputer. The presentation required a community of diverse individuals to solve a challenging chemistry problem. At the meeting volunteers were encouraged to bring their laptops to build a one-day instant supercomputer using bootable CDs that allowed them to work together in parallel.

COMP's instant supercomputer workshop provided the attendees the knowledge to construct an inexpensive research-level supercomputer and presented a unique opportunity to do "public science" to solve a current research problem with a real time audience, rather than disseminating prior results. Orlando Acevedo of Auburn University and Patrick Miller of D.E. Shaw Research LLC ran the workshop with four

goals in mind: (1) increasing minority participation in the COMP division, (2) increasing COMP's presence at regional meetings, (3) putting together an effective demonstration to raise the public awareness of computational chemistry, and (4) an outreach initiative to local Puerto Rican colleges and companies that could benefit from learning to build and use ad hoc computer clusters. Increased minority participation was realized, facilitated by leading the workshop in both English and Spanish. The workshop was highly successful and well attended.

Orlando Acevedo

2010 COMP Election Results

COMP Division Election News

During the 2010 elections, we had 419 (~20% of membership) ballots cast for the positions of Chair-Elect (2011), Secretary (2011-2013), and Councilor (2011-2013). The positions were filled by Jeffry Madura, Ed Sherer, and Emilio Esposito, with Patrick Lee elected as an Alternate Councilor. We would like to continue to increase the voter turnout for our upcoming 2011 elections happening this summer, so please look for an e-mail from COMP announcing the Survey Monkey based ballot. If you are consistently not receiving e-mail from COMP, make sure your e-mail address is current via www.acs.org.

For the 2011 elections, we will look to fill the positions of Chair-Elect (2012), Councilor (2012-2014), Treasurer (2012-2014), and Alternate Councilor (2012-2014). If you would like to participate in COMP as an officer, please let someone on the committee know of your interest.

Ed Sherer

Symposia for the Anaheim ACS National Meeting

The COMP Programming Board has a great program for the Spring ACS National Meeting in Anaheim (March 27th to 31th, 2011) that includes symposia for all areas of computational chemistry. COMP highlights of the Anaheim meeting include:

Newsletter of the COMP division of the ACS
Spring 2011, Anaheim

- ACS Award For Computers in Chemical and Pharmaceutical Research Award: Symposium in Honor of Thom Dunning
- Drug Discovery
- Materials
- Molecular Mechanics
- Mixing Quantum and Molecular Mechanics. My Mother Warned Me Never To Do This...
- Challenges in Industrial Computational Methods
- Docking and Scoring: A Review of Docking Programs
- Quantum Chemistry
- Computational Approaches to Spectroscopy Analysis
- The Computational Chemistry Component of Battery Research
- Poster Session (Sci-Mix, Chemical Computing Group Excellence Award, and Hewlett-Packard Outstanding Junior Faculty Award)
- A Tall Cool Session of Water
- Pioneers of Quantum Chemistry (HIST)
- Fragment and Local Orbital Methods in Electronic Structure Theory (PHYS)
- Quantum Information and Computation in Chemistry: Experiment and Theory (PHYS)

The poster session will take place on Tuesday evening in the Disneyland Hotel (South Exhibit Hall) near the convention center from 6 to 8 pm. The hotel is on the ACS shuttle route. 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.

2011-2012 National Meetings

In addition to our normal sessions, the Anaheim meeting (Spring 2011) will feature "Docking & Scoring: Review of Docking Programs" which is being organized by Neysa Nevins, Georgia McGaughey, and Greg Warren. The Denver meeting (Fall 2011) will feature a symposium dedicated to working with high throughput screening data "The cheminformatic aspects of high throughput screening: from the libraries, to the robots, to the models" and is being organized by Y. Jane Tseng.

Getting Involved with COMP Programming

All COMP members are welcome to attend the COMP Programming Meeting – Saturday, March 26th at 3pm in Room 201D of the Anaheim Convention Center – that takes place during every ACS National Meeting. The COMP Programming Board is always interested in having COMP members organize a symposium for an ACS national meeting. If you are interested in organizing or helping to organize a symposium for a future ACS national meeting, please contact Emilio Esposito. (emilio.esposito@gmail.com or 517.639.0684).

The COMP Programming Board is excited to welcome two new members: Michael Feig of Michigan State University and Eric V. Patterson of Truman State University. Michael's research is in the area of computational biophysics and focuses on implicit solvent models, protein-DNA complexes, protein structure prediction, and membrane bound peptides and proteins. Michael organizes the Membranes and Molecular Mechanics symposia (applications, force field development, methodology, and proteins). Eric is a physical organic chemist and his research applies the mathematics of quantum chemistry to understand properties and reaction mechanisms of organic molecules. Eric organizes the Quantum Chemistry (applications, DFT, and methodology) symposium.

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 Emilio for additional details.

Propose a Session for the National Meeting in Philadelphia

The Long Range Planning Committee of the ACS COMP Division is beginning to plan for the 244th ACS National Meeting in Philadelphia from August 19-23, 2012.

This is an opportunity for COMP ACS members to propose sessions of interest to you. If you are interested in organizing a symposium at the Fall 2012 Meeting, please submit a brief 1-page proposal *by Monday, August 22, 2011* to the COMP program chair, Emilio Esposito.

Chairing a session is a fun and rewarding experience which allows you to network with your colleagues in your field. It may also be considered a development opportunity for all scientists in any organization.

The proposal process includes identifying a subject area and a key speaker to provide background on the subject of interest, then recruiting a series of speakers working in the field from industry and/or academia.

Please take this opportunity to participate by sending your symposium proposal along to one of the committee members: Veerabahu Shanmugasundaram, Kate Holloway, Rommie Amaro, Emilio Esposito, Scott A. Wildman, and Melissa Landon. All contact information is given at the end of this newsletter with the exception of Melissa (melissa.landon@utoronto.edu) and Scott (wildman@biochem.wustl.edu).

Organize a Future COMP Symposium

Contact COMP Program Chair Emilio Esposito (emilio.esposito@gmail.com)

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 three HP Outstanding Junior Faculty Awards for outstanding tenure-track junior faculty at the Spring 2011 ACS National Meeting. The award provides \$1,000 to each faculty member.

The 2011 (Anaheim) winners are:

Wonpil Im, University of Kansas, "Transmembrane helix interactions in biological membranes"

Thomas F. Miller III, California Institute of Technology, "Exactly embedded density functional theory methods for the first-principles simulation of reactions in complex systems"

Ross Walker, San Diego Supercomputer Center "Towards routine microsecond molecular dynamics simulations of proteins on commodity hardware: Extreme GPU acceleration of Amber"

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)

Please see the COMP website for more details and due dates.

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 Anaheim 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 are:

- **Bin Zhang**: "Hydrophobically stabilized open state for the lateral gate of the Sec translocon," *California Institute of Technology*
- **Justin M Spiriti**: "Intrinsic bending flexibility of bare and protein-bound DNA by adaptive umbrella sampling on roll angles," *University of South Florida*
- **Sudipto Mukherjee**: "Development of the SB2010 testset to evaluate docking," *Stony Brook University*
- **Christina Bergonzo**: "Selective destabilization of lesions leads to divergent base flipping pathways by a DNA glycosylase," *Stony Brook University*
- **Ramu Anandakrishnan**: "N Log N generalized Born approximation," *Virginia Tech*

Applications for awards to attend the meeting in Denver, Co in August 2011 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 PACS system 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 in Anaheim

Tuesday, March 29 at noon

Are you interested to network with other COMP chemists and/or learn about what it's like to work in industrial and academic environments? Will you be attending the upcoming national meeting in Anaheim?

If so, make the most of your national meeting experience and join us for our COMP mentor lunches. Enjoy a free lunch and the opportunity to network!

Please join us in Anaheim, where we will offer an academic mentor lunch and an industrial mentor lunch on Tuesday, March 29 at noon. Groups will meet outside the COMP symposia and then depart for lunch at a local restaurant. Look for the signup sheets outside of the COMP symposia. Lunches are limited to the first 10 people who sign up.

As part of our ongoing initiative to bring computational chemists together and provide new venues for networking, COMP offers the possibility for junior members to have lunch with senior researchers at the national meetings. The goal is to allow for networking in an open, relaxed setting and to promote discussions about possible career paths in academia and industry. Academic mentees will be able to meet with professors and receive application and interview tips in time for the upcoming academic recruiting season. Industrial mentees can network and get the inside

scoop on what it's like to work in industry. All are welcome.

We also welcome and encourage COMP members to become part of the COMP mentor network as industrial or academic mentors. Please contact Rommie Amaro (ramaro@uci.edu) if you are interested in being a COMP mentor or with general questions about COMP mentoring initiatives.

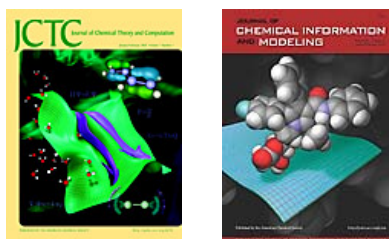
Journal of Molecular Graphics and Modelling



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 Jeffry D. Madura at Duquesne University and J. D. Hirst at University of Nottingham. The journal received an ISI Impact Factor of 2.169 in 2009.

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 # 2 in the Physics, Atomic, Molecular & Chemical category with an ISI Impact Factor of 4.804, up 12.4% from last year. It received 3,898 total citations in 2009, a substantial 54.4% increase over last year.

In the category of Computer Science, Information Systems, JCIM ranks #2 in citations with 8,973 total cites in 2009. The journal received an ISI Impact Factor of 3.882, the highest impact factor ever.

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

Annual Reports in Computational Chemistry (ARCC)

ARCC was instituted to provide timely, concise reviews of topics important to researchers in Computational Chemistry. It is published and distributed by Elsevier and sponsored by the American Chemical Society's Division of Computers in Chemistry (COMP). Members in good standing of the COMP Division receive a copy of the ARCC as part of their member

benefits. To ensure that you receive future installments of this series, please join the Division as described on the COMP website at <http://www.acscomp.org>.

Long-term COMP members will notice that topical sections within ARCC are constantly evolving to stay abreast of new developments in the field. Anyone interested in contributing to the production of future volumes of the ARCC, or anyone with new suggestions for topical subject areas should contact the Editor, Ralph Wheeler.

Ralph A. Wheeler, Editor

COMP Social Networking

Stay connected with ACS COMP by joining us and our members on LinkedIn or follow us on Twitter for the latest news @ACSCOMP. If you are interested in leading or joining a sub-group in LinkedIn to help organize networking events in your local region, please e-mail linkedin@acscomp.org.

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.

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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