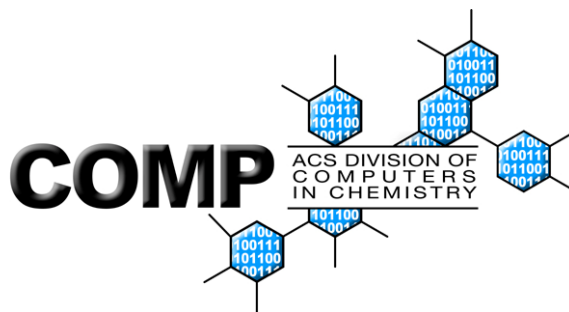


- Get involved with "COMP Together"
- CCG Student Excellence Awards, Peter Kollman Supercomputing Award, and HP Outstanding Junior Faculty Awards will be Presented On Tuesday
- Emerging Technologies Symposium to be Held On Wednesday



COMP Newsletter

Statement from the Chair

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

It's hard to believe how fast this year is flying by!

Just wanted to update you on what's been going on within the COMP division. As a member, you may not always be aware of what goes on behind the curtain, but we've been busy this year.

As I mentioned in the last newsletter, our program chair Emilio Esposito put together a great program for the Anaheim meeting. This included the Docking/Scoring challenge, in which many groups used a variety of commercial and academic programs on the same dataset and reported their results. There was also the award symposium for Thom Dunning, the 2011 winner of the ACS Award for Computers in Chemical and Pharmaceutical Research sponsored by Accelrys. Just as a reminder, if you didn't make it to the Anaheim meeting, you can still access recordings of these symposia on-line at the ACS web site.

And it looks like we will have another exciting program in Denver with wide-ranging topics for the organized symposia as well as many interesting contributed talks. The theme for the meeting is the Chemistry of Air, Space, and Water and we've got some of all of them, plus more,

on tap for you. There's everything from Battery Science to the Study of Water to extracting information from High Throughput Screening data and Protein-Ligand Interactions, not to mention the use of computational chemistry in Spectroscopic Analysis, Photo-Catalysis, and Photo-induced Charge Transfer Dynamics. As usual at the fall meeting, we will also announce the winners of the Chemical Computing Group Excellence Awards for students, the Peter Kollman Supercomputing Award for graduate students sponsored by The National Institute for Computational Sciences (NICS) and COMP, and the Hewlett-Packard Outstanding Junior Faculty Award. Be sure to attend the COMP poster session on Tuesday evening to see the awards presented. In addition, don't miss the Emerging Technologies in Computational Chemistry symposium competition sponsored by Schrodinger where you can find out about new computational tools on the horizon. As this award is decided based on talks given in the symposium, you can also root for your candidate and see if you agree with our judges' selection.

Many thanks to Carlos Simmerling who chairs the awards selection committee and to Curt Breneman who coordinates the selection of judges for the Emerging Technologies symposium.

I'd also like to take this opportunity to congratulate the COMP division members who were recently named ACS Fellows as part of the class of 2011 in honor of their involvement with the ACS as well as their commitment to science. The winning COMP members are highlighted in this newsletter.

We are currently putting together the program for the San Diego meeting this spring. I can tell you that it looks phenomenal so far. Don't forget that the deadline for abstract submission is November 1, 2011. We look forward to seeing many of you there, as it's typically one of the most well attended venues for the ACS. Maybe something about that great weather ... especially when those of us on the East Coast are often still enjoying those inevitable late spring snowstorms.

If you can't make it to any of the national meetings, give our local networking initiative, COMP Together, a try. 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. Thanks to Jane Tseng for developing the web-based tools. 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. Hanneke Jansen and the current local COMP Together champions have made big strides in enrolling members and getting events set up across the country. We currently have 320 people enrolled for notification of events and 17 champions who have started to work on planning events in 9 local areas. To learn more, see Hanneke's article on COMP Together in this newsletter. You can also use COMP Together to sign up for the academic and industrial mentor lunches for students that we sponsor at national meetings.

And don't forget about COMP on Facebook, LinkedIn, and Twitter (coordinated by Patrick Lee). We are also in the midst of revamping our web page, so stay tuned for a roll-out sometime this fall.

In addition, you should soon be receiving your copy of the Annual Reports in Computational Chemistry, edited by Ralph Wheeler, which offers an annual sampling of what's new in our field.

Last, but not least, you may recall our recent annual election of COMP officers (see this newsletter). Congratulations to all the winners and I look forward to working with them.

In closing, I'd like to thank all of our officers, symposium organizers, COMP Together champions, and other volunteers who keep our division running. Why don't you consider joining us? Many thanks also to our financial sponsors! And to all of our COMP division members who contribute to this enterprise in ways both large and small.

Please feel free to contact me with any questions, comments, or suggestions, or just to let me know how things are going in your little corner of COMP.
Thanks.

Kate Holloway
kate_holloway@merck.com

COMP Together

Networking Opportunities for COMP Division Members

The COMP Together initiative was launched in February of this year to facilitate gatherings of computational chemists on a local and informal level. There are currently 320 people signed up for notifications of events, and 17 champions who have started to work on planning events in 9 local areas. Kick-off events have happened in San Francisco, Boston, San Diego, and Bethesda, with an event in planning stages in New Haven. The COMP Together network is also being used to organize mentor lunches at the ACS National Meetings. Different areas have explored different formats for their gatherings including networking & seminar, happy hour, sit-down dinner & seminar, networking & several mini-talks, mentor lunch. The overall feedback has been very positive with great appreciation for both the networking and scientific exchange aspects of this initiative.

Getting involved:

- 1) Register for the COMP Together network and attend events of interest: http://www.acscomp.org/COMP_Together/reg_form.php
- 2) Help organize events: indicate your willingness to help out or to become a local champion on the registration form.
- 3) Propose new events or volunteer to be a speaker (in your local area or an area you're visiting). Proposals for presentations or new events should be sent to the local champions of the area you target for the event.
- 4) Sponsor this initiative with funds to cover meeting expenses. Contact the COMP treasurer or a local champion for a specific area you want to sponsor.

We hope to see you at one of our events!

The COMP Together Team
http://www.acscomp.org/COMP_Together/goal_contact.php

Hanneke Jansen

COMP Mentor Lunch

Join us Tuesday, 8/30 at noon outside of the COMP symposium. Attendees must sign-up through the COMP Together website.

ACS Fellows (COMP members)

The COMP Division congratulates the members of our Division who have been selected for the 2011 class of ACS Fellows (<http://cenm.ag/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:

Curt M. Breneman
Rensselaer Polytechnic Institute

Donald D. Clarke
Fordham University

Thom H. Dunning Jr.
University of Illinois, Urbana-Champaign

Andrew J. Holder
University of Missouri, Kansas City

Anton J. Hopfinger
University of New Mexico

Johanna M. Jansen
Novartis Institutes for BioMedical Research

Jeffry D. Madura
Duquesne University

H. Bernhard Schlegel
Wayne State University

C. David Sherrill
Georgia Institute of Technology

2011 COMP Election Results

COMP Division Election News

The COMP division elected three officers during the 2011 election held this summer.

Our Chair-Elect will be Kenneth Merz, and he will serve as COMP Chair during the 2013 calendar year. Ralph Wheeler was elected as Councilor with Veer Shanmugasundaram acting as Alternate Councilor. Running unopposed, Chris Harwell will continue to monitor the finances of COMP as Treasurer. We would like to thank Terry Stouch for participating in the election and for his continued support and interaction with the division.

As with previous elections, a ballot is being sent out via SurveyMonkey to email addresses listed under your ACS account. If you are not receiving these election notices, please make sure your contact information is up to date. If you are interested in participating with the COMP Division, or would like to run for an office, please get in touch with one of the current members of the committee.

Ed Sherer

Denver ACS Meeting

I want to thank all of COMP's organizers for the Denver ACS meeting for organizing another great set of COMP symposia.

The COMP Programming Board hopes those attending the Denver ACS Meeting enjoy the symposia that have been organized. Please peruse the technical program brochure (end of the newsletter) or visit the online version of COMP's technical program:

<http://www.acs.org/Denver2011>

-> Technical Program -> COMP.

I understand that not all of our members are able to attend all of the National Meetings. To provide access to National Meeting content, the ACS provides talks from the past two meetings online approximately a month after they are presented. I encourage

everyone to view presentations from this and past meetings at

<http://www.softconference.com/ACSchem/am.asp>.

One of the most common comments received by the COMP Programming Board regards abstract submission deadlines. Each meeting takes approximately eight months to organize. The fall meetings are always the most challenging because abstracts are usually due before the spring meeting has completed. In order to help you plan for the 2012 National ACS Meetings, the following abstract submission deadlines for COMP's technical program have been set.

San Diego (spring 2012, March 25-29, 2012)

Abstract submission closes: Tuesday, November 1st, 2011

Philadelphia (fall 2012, August 19-23, 2012)

Abstract submission closes: Tuesday, April 3rd, 2012

COMP technical program for the San Diego National ACS Meeting (March 25-29, 2012)

Abstract submission for COMP's technical program at the San Diego ACS meeting is now open – visit <http://abstracts.acs.org> to submit your abstract.

COMP technical program for the San Diego National ACS Meeting

The field of computational chemistry is ever expanding and the COMP membership is one of the most diverse in the ACS due to the wide scoping nature of our field. To reflect the heterogeneous character of the COMP division, the Contributed COMP Symposia include:

- Computational Approaches to Spectroscopy Analysis
- Computational Study of Water

- Data Science (Informatics)
- Drug Discovery (ADME/Tox, Ligand-based, Methodology, & Target-base)
- Materials Science
- Membranes
- Molecular Mechanics (Applications, Electrostatics & Polarization, Force Field Development, Methodology, and Proteins)
- Quantum Chemistry (Applications, Methodology, and Quantum Dynamics & Monte Carlo Simulations)
- Structural Bioinformatics
- The COMP Poster Session

The COMP division benefits from its active membership and this is evident by the large number of Member Organized Symposia for the San Diego ACS meeting. These symposia further demonstrate the diversity of our division. Please note that the following symposia are in most cases invitation only; please visit http://bit.ly/COMP_SanDiego_spring2012 for more information, before submitting an abstract to one of these symposia:

- Advancement of Computational Approaches in Pharmaceutical Solid State Chemistry
- Applications of Computational Methods to Environmentally Sustainable Solutions
- Collaborative Drug Discovery for Neglected Diseases
- Integrating Theory and Experiment for Discovering the Fundamental Chemistry of the Li-air and Other Metal-air Battery Systems
- Integration of Computer Simulation with Experiments

- Methods and Applications in Structure-based Design for Building Novel Molecules
- Molecular Simulations of Ligand-gated Ion Channels and the Mechanism of General Anesthesia
- Natural Product (Like) Scaffolds for Drug Discovery
- Perspectives in Applied Computational Methods
- Rational Drug Design
- Symposium in Honor of Andy McCammon

At each of the National ACS Meetings the COMP division provides the opportunity to have one's research highlighted through various symposia and awards. At the San Diego meeting the COMP Award Symposia are:

- The Thomas Kuhn Paradigm Shift Award (Talk)
- Chemical Computing Group Excellence Award (Poster)
- Hewlett-Packard Outstanding Junior Faculty Award (Poster)
- Peter Kollman Graduate Award in Supercomputing (Poster)

I believe that the COMP technical program presented at all ACS Meetings should "be by the members and for the members". If you are interested in organizing a symposium (currently accepting symposia for the Philadelphia, New Orleans, and Indianapolis national meetings) or presiding over a session, please contact me (emilio DOT esposito AT gmail DOT com; +1.517.639.0684; Skype: emilio.xavier.esposito) to discuss your idea for a symposium or volunteer your time to preside over a session.

Emilio Xavier Esposito
COMP Programming Chair

COMP Awards

COMP is proud to recognize excellence in computational approaches to chemistry with three different awards: the HP Outstanding Junior Faculty Award, the CCG Excellence Award, and the Peter Kollman Award in Supercomputing. Each awardee will present a poster at the Division's Tuesday evening poster session.

Applications for awards typically consist of a 2-page extended abstract, 2-page CV, 1-page personal statement, and a supporting letter. Please see the COMP website for more details.

<http://www.acscomp.org/Awards/index.html>

The application deadline for all awards is Monday, Oct. 17th by 5 pm EDT for the 2011 San Diego ACS Meeting.

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 2011 ACS National Meeting. The award provides \$1,000 to each of the four faculty members.

The 2011 (Denver) winners are:

Christine M. Aikens, Kansas State University, "Growth mechanisms of gold nanoparticles"

Jianhan Chen, Kansas State University, "Binding and folding of intrinsically disordered proteins: Nascent structures vs. intrinsic flexibility"

Elizabeth A. Amin, University of Minnesota, "New in silico strategies

toward the design of anthrax toxin countermeasures"

Alberto Striolo, University of Oklahoma, "Simulation-informed predictions of interfacial phenomena"

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 Denver meeting and provide a one-year software license of CCG's Molecular Operating Environment (MOE) for their academic groups (<http://www.chemcomp.com/>).

The awardees are:

- **John C. Faver**: "Estimation of error in energy functions for large molecular systems," University of Florida
- **Falgun Shah**: "Design and development of novel cysteine protease inhibitors of malaria parasite plasmodium falciparum: Virtual screening, de novo design, and combinatorial library synthesis," University of Mississippi
- **Maria P Frushicheva**: "Using computational enzyme design to study the promiscuous activities of phosphotriesterase and lactonase," University of Southern California
- **Wenkel Liang**: "Efficient first-principles electronic dynamics," University of Washington

- **Yi Shang:** “Simulations of spin-labeled HIV-1 protease exhibit diverse flap dynamics due to sequence polymorphism,” Stony Brook University

Peter Kollman Graduate Award in Supercomputing

The ACS Peter Kollman Graduate Award in Supercomputing has been created to provide supercomputer resources to outstanding students in the early stages of their graduate career, particularly for projects that need high performance computing resources for their chemistry-related project.

Winners (or their adviser, if necessary) will be the Principal Investigator of a new account on the “kraken” Cray XT5 supercomputer at the National Institute of Computational Sciences (NICS), with an allocation of computing time to support the project. For information about kraken, see <http://www.nics.tennessee.edu/computing-resources/kraken>.

The 2011 (Denver) winner is:

Robert Elder, University of Colorado

Journal of Molecular Graphics and Modelling

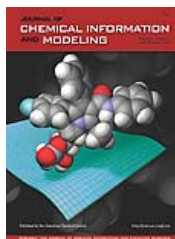


The *Journal of Molecular Graphics and Modelling (JMGM)* is devoted to the publication of papers on the uses of computers in theoretical investigations of molecular structure, function, interaction, and design. The scope of the journal includes all aspects of molecular modeling and computational chemistry, 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 2.033 in 2010.

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 received an Impact Factor of 5.138, up 6.4% from last year. Total citations in 2010 were 5,629, a substantial 44.4% increase over last year, based on recently released Journal Citation Report data from Thomson Reuters.

In the Computer Science, Information Systems category, *JCIM* ranks #2 in citations with 9,556 total cites in 2010. In addition, in the Computer Science, Interdisciplinary Applications category, the journal ranks #2 in impact with an Impact Factor of 3.822.

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

Emerging Technologies in Computational Chemistry

\$1000 prize sponsored by Schrödinger, Inc.

The Computers in Chemistry Division (COMP) of the ACS will hold our annual Symposium on Emerging Technologies in Computational Chemistry at the upcoming meeting in Denver on Sunday from 1:30 to 4:40 pm. 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.

To enter the competition for next year, please submit a regular short ACS abstract via <http://oasys.acs.org/> prior to the PACS deadline. It is also necessary to email a long (~1,000-word) abstract to the organizer. 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 PACS that cannot be part of the Emerging Technologies Symposium will be rescheduled in another appropriate COMP session at the Philadelphia 2012 meeting.

COMP Social Networking

Stay connected with ACS COMP by joining us and >600 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.

COMP Division Contact Information

Chair: M. Katharine Holloway
Merck Research Laboratories
Phone: (215) 652-7425
Email: kate_holloway@merck.com

Past Chair: Curt Breneman
Rensselaer Polytechnic University
Dept. of Chemistry
Phone: (518) 276-2678
Email: brenec@rpi.edu

Chair-Elect: Jeffry Madura
Duquesne University
Dept. of Chemistry and Biochemistry
Phone: (412) 396-4129
Email: madura@duq.edu

Secretary: Edward Sherer
Merck Research Laboratories
Phone: (732) 594-2883
Email: edward_sherer@merck.com

Assistant Secretary: Veerabahu Shanmugasundaram
Pfizer PharmaTherapeutics Research & Development
Phone: (860) 686-9264
Email: veerabahu.shanmugasundaram@pfizer.com

Treasurer: Chris Harwell
D.E. Shaw Research
Email: crharwell@yahoo.com

Assistant Treasurer: Sara Nichols
University of California, San Diego
Dept. of Chemistry and Biochemistry
Email: sara.nichols.w@gmail.com

Program Chair: Emilio X. Esposito
exeResearch LLC
Phone: (517) 639-0684
Email: emilio.esposito@gmail.com

COMP Award Coordinator:
Carlos Simmerling
Stony Brook University
Dept. of Chemistry
Phone: (631) 632-1336
Email: carlos.simmerling@stonybrook.edu

Newsletter: Orlando Acevedo
Auburn University
Dept. of Chemistry and Biochemistry
Phone: (334) 844-6549
Email: orlando.acevedo@auburn.edu

Web Support:
Y. Jane Tseng
National Taiwan University
Dept. of Computer Science and Information Engineering
Phone: +886.2.3366.4888#529
Email: yjtseng@csie.ntu.edu.tw

Editor, Annual Reports in Computational Chemistry:
Ralph Wheeler
Duquesne University
Dept. of Chemistry and Biochemistry
Tel: (412) 396-6341
Email: wheeler7@duq.edu

Coordinator of Educational Programs:
Michelle Francl
Bryn Mawr College, Dept. of Chemistry
Phone: (610) 526-5108
Email: mfrancl@brynmawr.edu

MPPG Liaison
Luke E. K. Achenie
Virginia Tech
Multiscale & Multiphys. Modeling Lab
Dept. of Chemical Engineering
Phone: (540) 231-4257
Email: achenie@vt.edu

Councilors & Alternate Councilors:

Ralph Wheeler
Duquesne University
Dept. of Chemistry and Biochemistry
Tel: (412) 396-6341
Email: wheeler7@duq.edu

Peter C. Jurs
Penn State University
Dept. of Chemistry
Phone: (814) 237-0098
Email: pcj@psu.edu

Carlos Simmerling
Stony Brook University
Dept. of Chemistry
Phone: (631) 632-1336
Email: carlos.simmerling@stonybrook.edu

Emilio X. Esposito
exeResearch LLC
Phone: (517) 639-0684
Email: emilio.esposito@gmail.com

Charles H. Reynolds
Johnson & Johnson Pharm-R&D
Phone: (215) 628-5675
Email: creynoll@its.jnj.com

Adrian Roitberg
University of Florida, Quantum Theory Project & Dept. of Chemistry
Phone: (352) 392-6972
Email: roitberg@ufl.edu

Rommie Amaro
University of California, Irvine
Health Sciences/Pharm. Sciences
Phone: (949) 824-2559
Email: ramaro@uci.edu

Patrick S. Lee
Eli Lilly & Co.
10300 Campus Point Dr.
San Diego, CA 92121
Email: patrick.s.lee@gmail.com