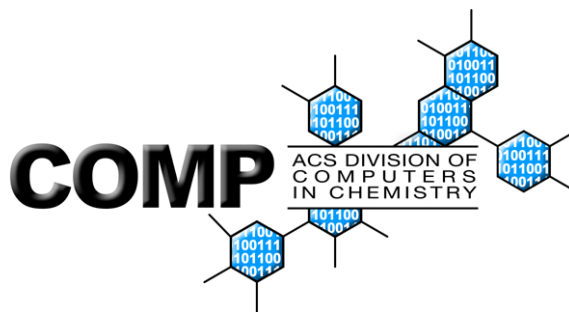


- COMP Nominated for a 2010 ChemLuminary Award
- Division's CCG Student Excellence Awards and HP Outstanding Junior Faculty Awards will be Presented On Tuesday
- Emerging Technologies Symposium to be Held On Wednesday



COMP Newsletter

Statement from the Chair

Curt Breneman, COMP Chair 2010, reports on the division's status

Dear Members of the Computers in Chemistry Division,

As 2010 Chair of the COMP Division, it's my pleasure to report that as a result of the efforts of our membership and those of our Executive Committee, the COMP Division has continued to excel at its mission of providing a wide variety of benefits to its members by providing networking opportunities, professional recognition through a variety of Divisional and National award programs, and strong symposium content at National ACS Meetings. This year has seen the addition of webcasting of a number of important symposia, including the Emerging Technologies in Computational Chemistry competition symposium (Sponsored by Schrödinger, Inc) that takes place each Fall. The vitality of our program is directly attributable to the generosity and foresight of our sponsors, whose contributions support the most important aspects of our mission, including symposium funds, grants and awards. Our newest sponsor, Accelrys, Inc., has just stepped forward to become the latest financial backer of the ACS Award in Chemical and Pharmaceutical Research for 2011 and 2012. The COMP Division Executive and Program Committees have set up a great

Fall ACS National Meeting in Boston, MA, and I look forward to seeing you there. I've been proud to have served the COMP Division as Chair in 2010 following a decade of service as Treasurer of the Division.

Curt Breneman

COMP Poster Session

Room Change

We had a last minute change to the location of the Poster Session on Tuesday Evening. The Poster Session is now located in the Grand Ballroom foyer on level 3 of the Boston Convention and Exhibition Center.

COMP is a 2010 ChemLuminary Award Divisional Finalist



The COMP Division has been selected as a 2010 ChemLuminary Award Divisional

finalist for "Recognition of Innovation and Outstanding Service to Members of a Division." In conjunction with the National Meeting in Boston, the 12th Annual ChemLuminary Award Celebration will take place on Tuesday, August 24, at the Westin Copley Place Hotel. The event begins with a poster session at 8 p.m. where Orlando Acevedo of the COMP division will present a poster of our activities. Recipients of the award will be subsequently announced and presented at the event.

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

ACS Fellows (COMP members)

The COMP Division congratulates the members of our Division who have been selected for the 2010 class of ACS Fellows (<http://pubs.acs.org/cen/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:

Wendy Cornell
Merck Research Laboratories

Christopher J. Cramer
University of Minnesota

Kenneth M. Merz Jr.
University of Florida

Charles H. Reynolds
Ansaris

Ralph A. Wheeler
Duquesne University

2010 COMP Election Results

COMP Division Election News

We are pleased to announce the outcome of the COMP officer elections held earlier this summer.

The 2011 chair-elect is Professor Jeffrey Madura. Professor Madura received his Ph.D. in chemistry from Purdue University in 1985 under the supervision of Bill Jorgensen. He is currently a full professor at Duquesne University, where he served as department chair from 2000 – 2010. His research interests include enhancement of water models, interactions of oligosaccharides with proteins, and monoamine neurotransmitters. Dr. Madura has also been involved with COMP for many years serving as program chair from 2007-2010.

The elected councilor for the 2011 – 2013 term is Dr. Emilio Esposito. Dr. Esposito received his Ph.D. from the department of chemistry and biochemistry under Jeffrey Madura. Dr. Esposito is currently a research scientist at exeResearch LLC, where he is focused primarily on structure- and ligand-based drug discovery. Emilio has been active in the COMP division since 2006, and he currently holds the position of program chair.

Dr. Edward Sherer will serve as the 2011 – 2013 COMP division secretary. Subsequent to pursuing master's studies in pharmaceutical sciences through a Fulbright scholarship, Dr. Sherer received his Ph.D. with Chris Cramer at the University of Minnesota. Currently, he works at Merck & Co, Inc. in Rahway, NJ where he provides modeling support to project teams and conducts research toward improving target selectivity. Ed has also served as assistant secretary of the COMP division.

Our new elected alternate councilor is Dr. Patrick Lee. Dr. Lee received his Ph.D. in computational chemistry from UCLA under the supervision of Dr. Ken Houk. He is currently a senior scientist at Eli Lilly and has previously served as alternate councilor for COMP.

We also acknowledge and thank the other candidates for office, including Veerabahu Shanmugasundaram and Daniel Ortwine. We thank our members for participating in the elections and look forward to working with our new officers!

Melissa Landon

Symposia for Boston ACS Meeting

Highlights for the Boston ACS Meeting

The COMP Programming Board has a great program for the Fall ACS National Meeting in Boston (August 22nd to 26th, 2010) that includes symposia for all areas of computational chemistry. COMP highlights of the Boston meeting include:

- Challenges in Industrial Computational Methods
- The Community Structure-Activity Resource (CSAR) Scoring Challenge
- Docking & Scoring
- An Emerging Challenge in Multiscale Modeling and Simulation: Mechanistic Understanding
- Emerging Technologies in Computational Chemistry
- Frontiers of Condensed Phase Theory and Simulation: A Tribute to Bruce J. Berne
- The PDB and Chemistry
- Scripting & Programming ("HPC on the Cheap" and "Cross Pharma Collaboration in High Performance Computing"; these are two separate symposia)

- Success Stories in Computer-Guided Chemistry
- Targeting Gram-Negative Pathogens
- Tautomers and Biology
- Using Waters Explicitly in Drug Discovery
- Poster Session (Sci-Mix, Chemical Computing Group Excellence Award, and Hewlett-Packard Outstanding Junior Faculty Award)

The poster session will take place on Tuesday evening in the Grand Ballroom foyer on level 3 of the Boston Convention and Exhibition Center. 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.

Some exciting changes have been made to the organization of the Boston meeting technical program. The traditional Molecular Mechanics and Quantum Chemistry symposia have been combined to create focused sessions. As computational chemistry expands to all areas of the physical sciences, (chemistry, molecular biology, biology, and material science to name a few) it is important that COMP's technical programming reflect these changing perspectives. At the Boston meeting there are dedicated symposia for colloids, materials, membranes, methodology, proteins, and water that include research from all areas of computational chemistry. This allows those attending the conference (speakers and audience) to see all aspects of a specific research area from several computational viewpoints.

The Boston meeting is the last meeting for Jeffrey D. Madura, as COMP's Programming Chair; Jeffrey has held this position since the Chicago National Meeting in the Spring 2007. He has provided graduate students and postdocs the opportunity to preside over Molecular Mechanics, Quantum Chemistry, and Drug

Discovery sessions, increased the diversity of the technical programming, and acquired private ballrooms for the COMP poster and award sessions. While we are sad to have Jeffrey step down as Programming Chair, he will stay active within COMP as the 2012 Chair-Elect and the COMP liaison and Co-Editor for the *Journal of Molecular Graphics and Modelling*.

Starting with the Anaheim, California meeting (March 27th-31st, 2011) Emilio Xavier Esposito, is the new COMP Programming Chair. Emilio has been an Assistant Programming Chair for the COMP Division since the Spring 2007 meeting and has organized the Molecular Mechanics, Quantum Chemistry, Drug Discovery, and Molecular Visualization symposia along with co-founding the "Scripting & Programming" symposium series. Additionally, Emilio is a councilor for the COMP Division and serves on the "Meetings & Expositions Committee" and "Technical Programming Subcommittee" along with being part of the PACS Advisory Board.

The COMP Programming Board welcomes Michael Feig (Molecular Mechanics Methodology, Force Fields, and Membranes), Melissa Landon (Quantum Chemistry Methodology), Y. Jane Tseng (Drug Discovery), and Scott Wildman (Drug Discovery) as organizers for future COMP programs.

2011 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. If you have an idea for a symposium that you would like to organize at either of these meetings, please contact Emilio (emilio.esposito@gmail.com or 517.639.0684).

Abstract submission for the Spring 2011

ACS National Meeting in Anaheim, California opens on Monday, August 23rd, 2010 and closes on Saturday, October 30th, 2010.

Getting Involved with COMP Programming

All COMP members are welcome to attend the COMP Programming Meeting – Saturday, August 21st at 3pm in Room 153C of the Boston Convention & Exhibition 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.

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.

Emilio X. Esposito and Jeffrey Madura

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 2010 ACS National Meeting. The award provides \$1,000 to each of the four faculty members.

The 2010 (Boston) winners are:

Alan Aspuru-Guzik, Harvard University, "Quantum information and quantum computation for chemistry"

John M. Herbert, Ohio State University, "Excited-state quantum chemistry for macromolecules and condensed phases"

Feng Wang, Boston University, "Mimicking coarse-grained simulations without coarse-graining: Enhanced sampling by damping short-range interactions"

Arjan van der Vaart, University of South Florida, "Information flow in biomolecules"

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 Boston 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:

- **Yat T Tang:** "Virtual screening targeting the PhoP response regulator to inhibit bacterial virulence," *Washington University in St. Louis*
- **Bonnie A Merchant:** "Computational investigation of the transport mechanism for monoamine transporters," *Duquesne University*
- **Roberto Olivares-Amaya:** "Quantum chemistry calculations for arbitrarily complex electrostatic environments: Benzene anion stabilization," *Harvard University*
- **Qin Cai:** "Biomolecular dynamics simulations based on the finite-difference Poisson-Boltzmann method," *University of California, Irvine*
- **Scott A. Johnson:** "Filtering and ranking enzyme designs using EDGE," *University of California, Los Angeles*

Applications for awards to attend the meeting in Anaheim, CA in March 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.

Journal of Molecular Graphics and Modelling

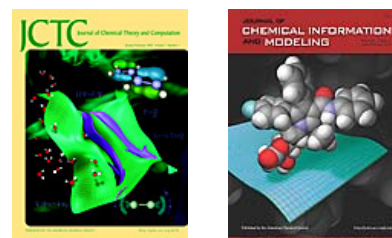


The *Journal of Molecular Graphics and Modelling (JMGM)* is devoted to the publication of papers on the uses of computers in theoretical investigations of molecular structure, function, interaction, and design. The scope of the journal includes all aspects of molecular modeling and computational chemistry, 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 2.169 in 2009.

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 # 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.

Annual Reports in Computational Chemistry (ARCC)

The COMP division is pleased to report that Volume 6 of *Annual Reports in Computational Chemistry* (ARCC) went to press on August 23, 2010 and will soon show up in your mailbox. Volume 6 features 14 outstanding contributions in six sections and includes a new section devoted to Nanotechnology and the re-emergence of the Chemical Education section. Topics covered (and Section Editors) include Simulation Methodologies (Carlos Simmerling), Quantum Chemistry (Gregory S. Tschumper), Chemical Education (George C. Shields), Nanotechnology (Luke E.K. Achenie), Biological Modeling (Nathan Baker), and Bioinformatics (Wei Wang). The articles in each section provide concise summaries of their respective topics unavailable anywhere else and are now indexed by the major abstracting services. The author's of each article and the Section Editors donated their time to make this volume of ARCC the highest possible quality and deserve a "thank you" from all of us!

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. Invitations are currently being issued for Section Editors for Volume 7 and volunteers will soon be solicited to author articles. So anyone interested in contributing to the production of Volume 7 of ARCC, or anyone with new suggestions for topical subject areas should contact the Editor, Ralph Wheeler, as soon as possible.

Ralph A. Wheeler, Editor

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 Boston on Wednesday from 1:30 to 5:30 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 Washington meeting.

240th National ACS COMP Sponsors

The COMP division would like to express gratitude to the following companies for their support of our programming at the 240th National ACS meeting.

- Pfizer
- Schrödinger
- Accelrys, Inc.
- Pharsight Corporation
- Chemical Computing Group
- Springer
- Chemaxon
- Dell
- Hewlett-Packard
- Thomas-Reuters
- RCHSolutions

COMP Social Networking

Stay connected with ACS COMP by joining us and >260 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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