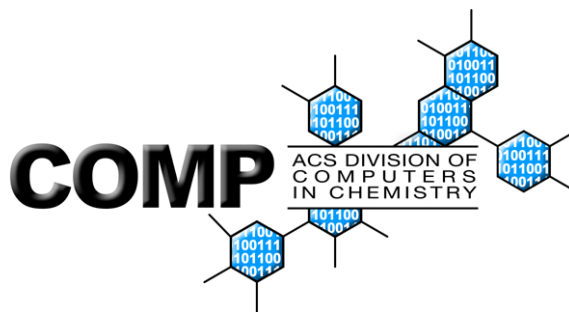


- Mark S. Gordon to be Honored Tuesday Afternoon with the ACS Award for Computers in Chemical & Pharmaceutical Research
- Robert G. Parr is the winner of the ACS Award in Theoretical Chemistry
- Division's CCG Excellence Awards and HP Outstanding Junior Faculty Awards to be presented on Tuesday Evening



COMP Newsletter

Statement from the Chair

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

This Newsletter may be the first you “see” of the COMP Division in 2009 but a lot of work has already been done. The COMP Division’s volunteer leadership team has finished a productive planning retreat which will have an impact on how we serve our membership. The common themes on which our efforts focus are the COMP community, scientific content, and divisional administration.

One of the Division’s goals is strengthening the community of computational chemists. This goal is particularly dear to my heart and very timely given the current economic situation. We hear from many of you that having a strong professional community is extremely important for getting support and advice, for access to information about job and career opportunities, for providing a platform to have scientific discussions and inspire each other. The COMP Division is working on tools and a network of local “champions” to facilitate COMP members to get together on a local and informal level. This can include events focused on science, networking, as well as mentoring activities for students and post-docs. The mentoring is something we have successfully been doing around the National Meetings in the form of mentoring lunches. This is again scheduled for Salt

Lake City. We want to thank Rommie Amaro for her leadership in setting up these mentoring lunches. Given their success, we are eager to try to provide this also on a local level. Look for information on how these efforts, that we have dubbed “COMP-together”, are coming along in future communications.

Another result of the planning retreat is a career symposium planned for the 2009 Fall Meeting in Washington DC, “Leaving the Nest: Life After Post-Doc’ing”. This is an interactive event, organized and introduced by Lisa Balbes, with panelists representing various career paths to answer questions and provide insights. Look for this in your program!

With respect to our focus on scientific content, we continue our strong commitment to the COMP programming at the National Meetings. Under the leadership of our Program Chair, Jeffry Madura, we continue to provide strong and multidisciplinary programming at the Spring and Fall National Meetings to benefit computational chemists worldwide. We also work to make selected multimedia content available on our website, www.acscomp.org. Check there for audio files and Powerpoint slides from the 2008 ACS Award Symposium for Computers in Chemical and Pharmaceutical Research, honoring J. Andrew McCammon.

The continued publication of *Annual Reports in Computational Chemistry* (ARCC) is another example of our commitment to provide access to top quality scientific content in our field. All members in good standing on the 2007 year-end list should have received volume 4 in the Fall of 2008. Volume 5 is in the making and all COMP members on the 2008 year-end list will receive this book later in the year. If resources permit, we will also include members joining during 2009 in the mailing of Volume 5 (your join-date will determine your rank on the list of those possibly included in the mailing, so join early). ARCC came into being under the leadership of David Spellmeyer. David was the sole editor for the first two volumes and from 2007 on has gradually shifted editorial responsibilities to Ralph Wheeler. We thank David for his dedication, leadership, and all his hard work on this publication. The Division received the 2006 ChemLuminary Division Recognition Award from ACS for its vision, commitment, funding, and strategic plan in creating the ARCC series. We also thank Ralph for his increasing commitment to this effort and congratulate him on taking sole responsibility as of Volume 5.

Divisional administration is something that is mostly behind the scenes from a membership perspective. It is critically important that we do not burn out our

volunteer leaders so we are continuously looking for new volunteers with skills and a passion to contribute to our community and share in the work involved in the various efforts as outlined above. Starting the year, we had a few vacancies, due to resignations. Our secretary, John Woolfrey, and one of our councilors, Andy Holder, resigned. John has embarked on a new career path and Andy is pursuing some other opportunities. We thank them for their service, which in the case of Andy also included many years as secretary and chair, and we wish them well. Emilio Esposito was the alternate councilor elected together with Andy, so he became the new councilor, leaving an alternate councilor position vacant. The executive committee made appointments to both vacant positions last month. We welcome Patrick Lee as the new alternate councilor, serving the remainder of Emilio's term (2009-2010). Patrick will be focusing on member outreach and communication, so you will definitely hear from him. We also welcome Melissa Landon as our new secretary, serving the remainder of John's term (2009-2010). We want to express many thanks to Ed Sherer, the assistant secretary, for stepping up to make sure all secretarial duties were taken care of and for supporting the executive committee.

Finally, our 2008 assistant treasurer, Chris Harwell, was elected to become treasurer, starting in 2009. We therefore have a vacancy for an assistant treasurer. Part of the duties for this individual would include supporting the COMP-together initiative, which has potential to grow into an effort where sponsorship monies would have to be received and distributed. If you are interested in discussing this opportunity, please contact me or Chris Harwell. Our contact information can be found on the COMP website and at the end of this newsletter.

In closing, I want to encourage you to contact any of us on the extended executive committee with ideas, comments, or suggestions for activities or resources that support COMP's mission: 1) to serve a diverse membership to lead the innovative use of computers in experimental, theoretical and computational chemistry and related chemical, physical and

biological sciences, 2) to support education, outreach, professional development and career growth, and 3) to provide venues to present, discuss, and publish research results.

Hanneke Jansen

Statement from the Past Chair

The past year was a productive one for the division, with delivery of strong programming at the national meetings, another fine volume of *Annual Reports in Computational Chemistry*, and other member benefits such as the mentor lunches. When I first became active in division leadership back in 2001, the main member benefit was the programming at the national meetings, so it has been very satisfying to be involved with the development and launch of these additional benefits in the intervening years. And current Chair Hanneke Jansen is laying the foundation to establish additional benefits to help members communicate and network more effectively.

Despite the success of these ongoing ventures, the year was not without its surprises! Many of you either will have experienced firsthand or heard about the logistical problems experienced by COMP at last year's fall meeting in Philadelphia. I would like to take this opportunity to explain what the problems were, our understanding of how they came about, and what we did to address them in the short and long term. These problems arose from a last minute relocation of our sessions from the Convention Center, our traditional home, to a hotel located some distance away. We were told this relocation occurred when the Philadelphia Convention Center informed ACS that the space reserved for COMP would no longer be available due to construction in that area.

This last minute change had two major effects. First, room assignments at the hotel were not appropriate. These assignments are normally made well in advance by ACS based on attendance estimates provided by division program chairs for each scheduled session. Fortunately, the ACS operations staff person assigned to the hotel was very

responsive and we were able to change the room assignments on-the-fly and minimize inconvenience. A further complication came from the way the rooms were furnished. The chairs had high backs and the screens were fixed relatively low on the wall. Unfortunately, nothing could be done about that. The second effect of the relocation was that the technical sessions and people attending them were far removed from the Exposition.

Under normal circumstances, when COMP sessions are located in the Convention Center in a given city, members can alternate attendance at technical talks with visits to the vendor booths at the Exposition. The remote location of the COMP sessions in Philadelphia led to greatly reduced traffic at the vendor booths at the Exposition, including the software vendor booths. The division leadership was distressed to hear of this problem, since the division has long enjoyed a strong relationship with many of these vendors. Their employees are often themselves division members who organize or participate in our technical sessions. Further, the companies provide much appreciated financial support for division awards, symposia, and activities such as mentor lunches.

We want you to know that after addressing the immediate problem in Philadelphia, i.e. the room assignments, division leadership followed up with multiple groups within ACS. We communicated the details of the problem and its impact on technical session organizers and attendees and division sponsors. We also explored strategies for avoiding this problem in the future.

ACS is a big organization and not all offices and committees were equally responsive. One group that was particularly supportive was the Department of Division Advancement, which is committed to the ongoing health and success of COMP and other divisions, and we would like to thank them.

Program Chair Jeffry Madura provided an update on the situation. "ACS has responded by establishing a liaison for the Salt Lake City (SLC) meeting and we are going to push for this continued

communication with them. The ACS has also given us a good spot for SLC." Jeffrey has also emphasized the need for COMP to be co-located with divisions such as CINF, PHYS, and MEDI, and this should further help to anchor us in a convenient location.

The ACS national meetings will always be huge undertakings and some logistical problems are to be expected. The May 12, 2008 edition of *Chemical and Engineering News* contained a contribution by ACS Council Committee on Meetings and Expositions Chair Willem Leenstra explaining why relocating entire national meetings is sometimes necessary.

<http://pubs.acs.org/subscribe/journals/cen/86/i19/html/8619comment.html>

We are confident that the problems experienced in Philadelphia were an anomaly and are doing our best to work with ACS to avoid such a situation in the future. Many people are committed to the successful planning and execution of the COMP sessions at these meetings, so it is useful to consider the things that do go well! For example, in recent years a private room was made available for our Tuesday evening poster session to provide a better setting for the CCG and HP awards ceremonies. We are grateful for that. We are also thankful to ACS Meetings Associate Reggie Washington, who works with the COMP Program Chair and Treasurer to set up the Poster Session and Awards Ceremonies. So that you can get to know Reggie better, we have included a photo and Q&A elsewhere in this newsletter.

Wendy Cornell

COMP Elections Summary 2008

Elections in 2008 were conducted electronically using the online system Survey Monkey. The survey link was sent out via the active COMP member's email list so if you did not see an email concerning the election or did not see the election announcement on the COMP website (<http://www.acscomp.org>) please inform the division.

The Chair-Elect position was filled by Curt Breneman who has previously served as the Treasurer for COMP. Chris Harwell who had been Assistant-Treasurer was elected to the position of Treasurer. One open Councilor's position was filled by Ralph Wheeler, who will hold that position until 2011. Finally, the 2009-2011 Alternate-Councilor position was filled by Chuck Reynolds. Both Ralph and Chuck have held positions in COMP previously.

With the vacancy of one Councilor's position in 2008, Emilio Esposito was transitioned from Alternate-Councilor to the position of Councilor. Recent appointments made at the 2009 Executive Planning Meeting include Patrick Lee as Alternate-Councilor, and Melissa Landon as Secretary.

Currently COMP has the Assistant-Treasurer's position open, if you are a COMP member and have interest in volunteering, please inform the committee.

Ed Sherer

Symposia for Salt Lake City ACS Meeting

Highlights for Salt Lake City and preview of the Washington D.C. ACS Meeting

The Spring 2009 American Chemical Society Meeting in Salt Lake City promises to be interesting as this is the first time the city has hosted the event. A number of COMP symposium organizers have scheduled a variety of topics ranging from high-performance computing and advanced computational methodology to applications in nanomaterials and drug discovery. If you have any ideas or would like to organize a symposium for a future national meeting please contact Jeffrey Madura at madura@duq.edu.

- Advancing Computational Chemistry through High-Performance Computing: From the Workstation to Petascale and Beyond: Michael Dewar Memorial Symposium (S.T. Brown, R.C. Walker, T.E. Cheatham III)

- Molecular Modeling in Chemical Processes (L. Achenie)
- Connecting Computation to Experiment using Combined QM and MM Methods (B.P. Krueger, R.C. Walker)
- Nanomaterials Modeling and Informatics (C.M. Breneman)
- Molecular Mechanics (E.X. Esposito)
- Drug Discovery (I. Visiers, Z. Yang)
- Quantum Chemistry (A. Roitberg)
- ACS Award for Computers in Chemical and Pharmaceutical Research: Symposium in Honor of Mark S. Gordon (M.S. Gordon)
- Hewlett-Packard Scholar Awards (C. Simmerling)
- Chemical Computing Group Excellence Award (C. Simmerling)
- Poster Session

The poster session will take place on Tuesday evening. The CCG Student Excellence Award and the Hewlett-Packard Outstanding Junior Faculty Award will be presented at that time. The COMP division would like to acknowledge the generosity of our sponsors who provide funding for selected symposia and the poster session.

A number of symposia are in place for the Fall 2009 meeting in Washington D.C. Symposia:

- Computational Chemistry in the Discovery & Development of Novel Anti-Infective Agents (G.S. Weston, R.J. Czerminski, J.I. Manchester)
- Protein Dynamics and Function (H.-X. Zhou, G. Hummer)
- Scripting & Programming (J.M. Leonard, J.R. Hammond, C. Harwell, R.E. Amaro, R. Guha, E.X. Esposito)

- Simulation of (Bio)Organic-Inorganic Interfaces and Nanostructures Using MD, MC, and Multiscale Approaches (H. Heinz)
- Structure Activity Relationship Knowledgebases (E. Bolton)
- The Role of Quantum Chemistry in Chemical Biology and Medicinal Chemistry (A.M. Ferreira)
- Molecular Visualization (R.E. Amaro, E.X. Esposito)
- Emerging Technologies (C.M. Breneman)
- Leaving the Nest: Life after Post-Doc'ing (L. Balbes)
- Poster Session
- Chemical Computing Group Excellence Award (C. Simmerling)
- Hewlett-Packard Scholar Awards (C. Simmerling)
- Quantum Chemistry (A.E. Roitberg)
- Molecular Mechanics (E.X. Esposito)
- Drug Discovery (I. Visiers, K.E. Gubbins)

“ACS Profiles” – Mr. Reginald Washington

The ACS national meetings are huge undertakings, typically attended by 10,000 to 18,000 people and supported by an extensive cadre of ACS paid staff and volunteers. In this section we introduce readers to one of those staff members - Reggie Washington. Reggie has worked behind the scenes for many years with the COMP program chairs and treasurers to make the Tuesday evening poster session and associated CCG and HP award ceremonies a success. Be sure to say "hello" – and "thanks!" – the next time you see him.



Q) How long have you worked for ACS?

A) I first worked for ACS as a contractor during 1998-1999 and then returned as a permanent employee in 2000.

Q) Where are you from originally?

A) I was born in Lincoln, NE but raised in Clinton, MD. My father was in the Air Force.

Q) What are your responsibilities at ACS?

A) I am a Conference Associate and EMS (Event Management System) Administrator

Q) What do you like about your job?

A) It's never the same day twice. I love it. I have a great team of people that I work with. I enjoy coming to work.

Q) The national meetings must be very busy for you and your colleagues. What is that like?

A) The week before is very busy and kind of festive. We have pep rallies and people hold last minute meetings. We pack the trunks to ship out. Closer to the start day it gets really quiet at ACS HQ since people are disappearing. Once we arrive at the national meeting it is very fast paced. When you get there you have one day of rest and relaxation and fun. After that you are constantly busy. There is always something to do, especially at the Convention Center.

Q) COMP relies on you to help set up the Tuesday evening poster sessions. How would you compare us to other divisions?

A) I really know what COMP needs. You are the one poster session that, when I see

it, I know we need the (CCG and HP) award winners up front, you need a podium, etc. You guys never change, which makes it easier for me. I know what you need to make it successful. I get to know the COMP program chairs and I've built friendships with some of you. It seems like you guys have a nice group.

Q) The Fall 2008 meeting in Philadelphia was unusually complicated for COMP, with the last minute change from the Convention Center to a hotel. How was that meeting for you?

A) In Philadelphia there was always a surprise around the corner. I would think I had my grip on something and then would lose it.

Q) Do you ever look at the COMP posters?

A) Yes, I skim through them, but there are so many I can't remember them. Sometimes I see something neat. I haven't studied much chemistry myself -- I am going to school for hospitality services management at Prince Georges Community College.

Q) What do you like to do when you are not at work?

A) I am into sports like flag football and I just returned from a tournament. Otherwise I watch sports -- football, basketball – and I just chill with my family.

Interview by Wendy Cornell

ACS Award for Computers in Chemical & Pharmaceutical Research

Sponsored by Schrödinger

SCHRÖDINGER

Professor Mark S. Gordon of Iowa State University is the winner of the 2009 ACS Award for Computers in Chemical and Pharmaceutical Research for his contributions to the field of Quantum Theory.

Dr. Gorden received his B.S. degree at Rensselaer Polytechnic Institute and his Ph.D. degree from Carnegie Mellon University. After three years as a postdoctoral associate at Iowa State University, Dr. Gorden joined the faculty at the North Dakota State University for 22 years until he moved in 1992 to his current appointment at Iowa State University.

Professor Gorden will present his award address "Toward a comprehensive method for intermolecular interactions" before the COMP Division on Tuesday afternoon. This award is generously sponsored by Schrödinger.

ACS Award in Theoretical Chemistry

Sponsored by Dell Incorporated.



Professor Robert G. Parr of the University of North Carolina is the winner of the 2009 ACS Award in Theoretical Chemistry. His work has advanced the knowledge of density functional theory.

Dr. Parr received his A.B. degree at Brown University and his Ph.D. degree from University of Minnesota. Parr joined the faculty at the University of Minnesota from 1947-48. In 1948 he moved to the Carnegie Institute of Technology (now Carnegie-Mellon University) until 1962 when he moved to John Hopkins University. In 1974 Dr. Parr moved to the University of North Carolina at Chapel Hill.

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

*Apply for the COMP Division's
CCG Student Excellence Award
or HP Outstanding Junior
Faculty Award*

More information at:
www.acscomp.org

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 five HP Outstanding Junior Faculty Awards that provide \$1,000 in travel funds, a special gift from Hewlett-Packard, and recognition at the COMP poster session awards ceremony in Salt Lake City to each of the four outstanding tenure-track junior faculty selected.

The Spring 2009 winners were:

Aurora Clark, "Force-field development for heavy elements using ab initio data and the force matching method", Washington State University, Pullman, WA

Aaron Dinner, "Enhanced sampling methods for molecular systems far from equilibrium", University of Chicago, Chicago, IL

Alexey Onufriev, "A new generation of analytical tools for biomolecular electrostatics", Virginia Tech, Blacksburg, VA

Edward Valeev, "Practical many-body methods for computational thermochemistry, kinetics, and spectroscopy", Virginia Tech, Blacksburg, VA

The Awards are designed to assist new faculty members in gaining visibility within the COMP community. While special consideration will be given to Assistant Professors presenting work in the area of algorithm and methods development, applications are invited from all current tenure-track junior faculty who are members of ACS and the ACS Division of Computers in Chemistry. Postdoctoral researchers in transition to faculty appointments may also be considered.

Selection criteria will include the novelty and importance of the work to be presented, as well as the level of Departmental support as indicated by a letter of support by the Chair or Chair designee.

To apply for an award for the 239th ACS National Meeting in San Francisco, CA, March 21-25, 2008, an extended abstract of the work (no more than 2 pages), a CV, and the letter of departmental support should be sent to **Carlos Simmerling** as a pdf or text file at: carlos.simmerling@gmail.com.

Chemical Computing Group (CCG) Excellence Awards



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 Salt Lake City meeting and one-year software license for the CCG Molecular Operating Environment (MOE).

<http://www.chemcomp.com/>

The awardees, in alphabetical order, are:

- Jiahao Chen, University of Illinois at Urbana-Champaign, "Investigating the properties of new water models capable of polarization and intermolecular charge transfer"
Advisor: Todd Martinez
- Wenxun Gan, University of Chicago, "Estimating transition rate and free energy of Src kinase activation using Markov state model"
Advisor: Benoit Roux
- Dian Jiao, University of Texas at Austin, "Calculation of protein-ligand binding free energy by a

polarizable force field"
Advisor: Pengyu Ren

- Kelly Lancaster, Georgia Institute of Technology, "Intramolecular electron transfer in two- and three-center mixed-valence triarylamine"
Advisor: Jean-Luc Brédas
- Yilin Meng, University of Florida, "Constant pH replica exchange molecular dynamics simulation in biomolecules"
Advisor: Adrian Roitberg

Applications for awards consist of an extended abstract, CV, personal statement, and a supporting letter from the student's advisor and are due to **Carlos Simmerling** at carlos.simmerling@gmail.com. In addition, an abstract for the scientific presentation must be submitted in the CCG awards COMP section of the ACS OASYS system (<http://oasys.acs.org/oasys.htm>) for online submissions prior to the deadline for the meeting at which the awards will be presented. Submissions are restricted to North, Central and South American students. Please see the COMP website for more details.

Join the COMP Division

Become a new COMP Division member or change your membership status by using the on-line form or calling 800.333.9511.

Membership dues are:
ACS Member \$15.00
Student Member \$7.50
Retiree \$15.00
Division Affiliate \$17.00
National Affiliate \$17.00
Outside US, add \$3.00 for postage

COMP Social Networking

Join us on any one of our social network sites for latest news and to participate in discussions. You can request to join our network by going directly to the websites.

Facebook:

<http://www.facebook.com/group.php?gid=13754117515>

Linkedin:

<http://www.linkedin.com/groups?gid=1819163>

For additional information regarding joining us on the web, please e-mail: linkedin@acscomp.org

or

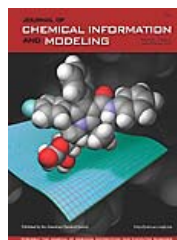
facebook@acscomp.org

Journal of Molecular Graphics and Modelling



The *Journal of Molecular Graphics and Modelling* (JMGM) is doing well with a steady and increasing stream of submissions. The Journal publishes 8 issues per year with an ISI Impact Factor of 1.932. The journal is edited in the United States by Andy Holder. COMP is pleased to be associated with JMGM and encourages its members to solicit submissions to the journal.

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 ranked in the top 20 in Multidisciplinary Chemistry with an ISI Impact Factor of 4.308. It received 1,526 total citations in 2007.

In the category of Computer Science, Information Systems, *JCIM* ranks #2 in citations with 7,113 total cites out of 92 journals in that category. The journal received an ISI Impact Factor of 2.986.

ACS ProSpectives



Discovery & Selection of Successful Drug Candidates with special emphasis on Structure-Based Drug Design

April 26 – 29, 2009 in Boston, MA at the Cambridge Hyatt

Structure Based Drug Design Program

- **Keynote:** Peter Mueller of Vertex
- Mike Palmer of Pfizer (UK) on PDE5
- Matt Weiss of Amgen on BACE Inhibitors
- Graham Johnson of RibX on Radezolid
- Vadim Dudkin of Merck
- Joseph Kim of Amgen on b-Raf
- Christopher J. Helal of Pfizer on PDE10A Inhibitors

ALSO:

- Keynote by **Magid Abou-Gharbia** of Temple University, recently retired VP of Wyeth
- Half day sessions will be held on blood brain barrier permeability

and PK/PD successful transitions to the clinic

- **Scott Biller** of Novartis, **William Greenlee** of Schering Plough, **Terence Kelly** of Boehringer-Ingelheim and **Alan Palkowitz** of Eli Lilly will give presentations on small molecule drugs that have been discovered and advanced through proof of concept, or been successfully marketed by their companies -- how the compounds were discovered, lessons learned, and how those lessons were instituted into their company's drug discovery processes

Please check www.acsprospectives.org regularly to obtain the most complete, up-to-date information available on all 2009 conferences, including confirmed speakers and abstracts as they become available.

If you have any questions, please email acsprospectives@acs.org or call 1-800-227-5558 and ask for ACS ProSpectives.

How can COMP reach you?

Updating your contact information.

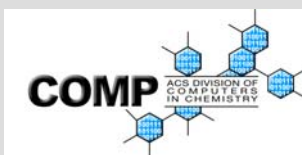
Communications and benefits from the COMP Division to its members sometimes disappear in a void due to incorrect or outdated addresses. Items of importance and value include the COMP elections and the *Annual Reports in Computational Chemistry* (ARCC). The elections have been held electronically over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

You can check and change your address(es) on-line by logging in to the

COMP Mentor Lunches

Make the most of your annual meeting experience and join us for our COMP mentor lunches in Salt Lake City. Groups *will meet outside the COMP symposia at noon on Tuesday*, then depart for lunch at a local restaurant. Look for the signups outside the COMP symposia.

Enjoy a free lunch and the opportunity to network!



Sponsored by COMP and BioSolvIT



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.

Emerging Technologies

\$1000 prize to be awarded at the 238th ACS National Meeting, Washington, D.C.

The Computers in Chemistry Division (COMP) of the ACS will hold the eighth annual Symposium on Emerging Technologies in Computational Chemistry at the American Chemical Society National Meeting, Washington, D.C., August 15-20, 2009. 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.

All are invited to participate. To enter the competition, please submit a regular short ACS abstract via <http://oasys.acs.org/> prior to the OAsys deadline (believe it or not, OAsys opens for the Washington, D.C. meeting on January 19th). 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 OASYS that cannot be part of the Emerging Technologies Symposium will be rescheduled in another appropriate COMP session at the Washington meeting.

COMP and CCL

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

Information about upcoming COMP events will be distributed via this CCL.

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