Spring 2006 Highlights

- COMP Wins 2005 Divisional ChemLuminary Award
- Thomas Kuhn Paradigm Shift Award; New for 2006
- COMP member drive; advantages of membership

COMP Newsletter

Statement from the Chair

Jeffrey D. Evanseck, COMP Chair 2006, reports on the Division status

The COMP executive committee gathered in Pittsburgh this year for the 2006 strategic planning retreat. It is at this annual event that the executive committee members volunteer a full weekend of time to chart the course of next year's activities. All of the committee's energy goes into increasing the quality and number of benefits for COMP membership.

The strategic planning retreat was intense, and full of great ideas. The agenda was set by the activities from the previous year and newly suggested items to maintain our strong programming of symposia and bring new and needed benefits to the membership. To help identify the needs of the Division, we created an on-line survey last fall. When asked about what new activities you would like to see from COMP, over 30% of you indicated that you would like to see (1) more email communication, (2) more graduate awards and (3) more involvement at regional and local levels.

The electronic communication with the membership has always been plagued with problems. First, the email list maintained by national is frequently inaccurate. Second, many people feel overwhelmed with the sheer volume of email received on a daily basis. Finally, it takes hardware and human resources to maintain the monthly email list changes that would be difficult for COMP to take on without additional volunteerism. Last year, we thought we resolved the communication problem by establishing the Computational Chemistry List (CCL) as our Division's mode of electronic communication. However, we are discovering that this is not the most effective mode to reach our membership. We do find that we connect very well with our younger and student members by using the CCL. Thus, the CCL will not be abandoned, but new communication avenues will be explored.

Our plan is to test the idea of using a listserve to better communicate with the bulk of the membership. A listserve will be initiated by using a corrected email list provided by national. We will advertise on the COMP website and at the COMP poster session in Atlanta to get the membership to join and improve the accuracy of the list. If you do not receive a welcome message from us, then please visit our website (http://membership.acs.org/C/COMP/) to correct your email address. Thank you Lisa Balbes for taking care of this entire process!

The plan is to communicate with the membership a few key times a year. We will send important information and reminders to you before each national ACS meeting and after each annual strategic planning retreat. Other COMP news involving local and regional events involving COMP, webpage changes, and awards will be sent as the occasions arise. Let us know what else you would like to be informed on! We hope that communication of this type and frequency will bring the membership up to date and inspire a more active infusion of ideas into the direction of our Division.

We have been informed by national, that electronic elections are right around the corner. It is not clear how fast the transition will occur, but please expect to elect your COMP Executive Committee on-line in the near future. This is another reason why we must sort out the email mailing list and maintain its accuracy. As we receive more information on electronic elections, we will pass it along using the listserve, as described above.

The Chemical Computing Group (CCG) continues to sponsor the graduate student travel awards for each national meeting (http://www.chemcomp.com/). It was decided last Fall that CCG would support five graduate student travel awards per meeting. Each award winner will receive a check for $1,150 to support the student to attend and present their research in the COMP poster session or as an oral presentation. In addition, the research advisor of the winning student receives a license for the Molecular Operating

Environment (MOE) software for research purposes. Please note the deadline for applications is usually a few weeks before the normal COMP deadline for each national meeting. Andrew Good (CCG Excellence Awards Coordinator) is managing the review of applications and coordination with CCG and should be contacted regarding any questions. The awards provided by the CCG are an excellent benefit to our membership. We continue to search for other novel ideas to bring younger members into our Division. If you would like to be involved, or have new ideas, then please let us know.

Over the last year, the Division has been getting involved with regional and local activities. Phil Bowen is the Division's new coordinator of local and regional events. On September 15, 2005 the Philadelphia Local Section and COMP co-sponsored an evening flashmob workshop. Sixty attendees enjoyed a social hour, traditional Philadelphia hoagies and watched real science happen. A flashmob cluster from fifteen laptops was built and ran a 10 picosecond molecular dynamics simulation of a protein complex. Participants included ACS local section members; COMP division members; local college faculty, graduate and undergraduate students in chemistry, biology, physics and computer science and high school teachers and students. Dr. Patrick Miller of Lawrence Livermore National Laboratory gave a talk about ad hoc cluster computing, followed by a lively discussion period. Attendees went home with a t-shirt, and those who wished to set up their own clusters with the cables and CDs to do so.

Michelle Francl (2004 Chair) recently wrote that this was an opportunity to do "public science", to solve a research problem with a real time audience, rather than presenting previous results done tucked away in a laboratory. The opportunity to participate in actual research generates excitement among students and the general public, and raises public awareness of the chemical enterprise. The event highlighted the multidisciplinary connections chemists can make and use, showing how collaborations between computer scientists and chemists can make new science happen. Attendance by computer scientists and physicists offered expanded possibilities for networking for chemists, as well as encouraged the reach of society into areas we usually do not reach.

One of the biggest benefits brought to the COMP membership over the last year was the successful publication of Volume 1 of the Annual Reports in Computational Chemistry (ARCC). David Spellmeyer (ARCC Editor) masterfully spearheaded this journal to bring value added to COMP membership. The first volume, published in March 2005, consists of six sections: Quantum mechanical methods and applications, molecular modeling methods, advances in QSAR/QSPR, applications of computational methods, chemical education, and emerging science. The first volume contains an extensive index with 18 articles, spanning a full range of thematic topics. The intention is to run a cumulative index for all volumes, enabling members to identify all reports published on a given topic quickly. Thus, members will gain maximum benefit from having received several volumes through their continued membership in COMP. The second volume is now complete and has been sent to the printers. You should receive your copies in the mail later this year. If you would like to contribute as an author in Volume 3, then please contact David as soon as possible. The last piece of news on the ARCC is that Ralph Wheeler will co-edit the ARCC over the next volume, before he takes over the full responsibility.

The COMP Division continuously evaluates and improves its symposium programming. Wendy Cornell (Programming Chair) has done an outstanding job in creating a great series of symposia over the last few years. One component of this is her attention to multidisciplinary topics. The Division hosts and engages in active co-sponsorship with several other divisions on a regular basis. In 2005, we co-sponsored 17 symposia with a total of 7 other divisions: PHYS, CINF, CHED, MEDI, PROF, NUCL, AGRO. The division has also recently begun targetted recruiting of session chairs for the three General Oral session tracks at the national meetings -- Drug Discovery, Molecular Mechanics and Simulation, and Quantum Chemistry. In the past, this session chair function was seen as a necessary obligation to be carried out by the program chairs and other members of the Executive Committee. Some of the perks that the Committee is using in the "re-branding" of these positions is the opportunity to get visibility for our younger members and an opportunity to contribute to the division and our profession. We have also been able to secure corporate sponsorship for some of these sessions to provide refreshments. One final note is that Jeffry Madura will transition in as the Programming Chair, when Wendy finshes three years of service at the Fall San Francisco meeting this year.

Feedback is critical to our success, and we need the membership to get involved. At the Tuesday evening poster session in Atlanta, we will have a short questionnaire for you to fill out. Please locate it near the CCG winner posters. This will help the Division to keep its competitive edge in being proactive and innovative in improving benefits to its membership. I strongly encourage you to respond and help refine the direction of your Division.

Finally, please realize that we need your help. We have a number of appointed positions with the Executive Committee that need to be filled. If you want to get involved, then please contact me as soon as possible. Our email addresses are listed within the newsletter and posted at our website. We look forward to hearing your ideas on how the Division can be further improved!

Jeff Evanseck

Statement from the Past Chair

Continuing upon a great year

First, I would like to thank the members of the Division for supporting me this past year in all of the activities we have undertaken. I would especially like to thank the special group of people that have served on your Executive Committee. They have given their time and attention to conducting the business of the Division. They have been an inspiration, and it has been a

privilege to lead such a group. They serve you well. A great deal was accomplished last year, but there is much to be done. I will say that my experience as Chair shows me that our Division is one of the best organized and effective of any in the ACS. Please support Jeff Evanseck this year as we move forward yet again.

Andy Holder

COMP Wins 2005 Divisional ChemLuminary Award

All of the hard work is paying off. Your COMP Division was awarded the coveted 2005 Divisional ChemLuminary Award at the fall National ACS Washington D.C. meeting! 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 involved the assembly of a supercomputing "flashmob" last year at the Fall National ACS Philadelphia meeting. Briefly, commodity laptops or desktops can be temporarily linked together to achieve supercomputing speeds. The ingredients are easy; we can provide all of the necessary software and information on the cables required. To find out more about our flashmobs, see (http://membership.acs.org/C/COMP/flashmob.html). Michelle Francl (2004 Chair) and Pat Miller (Flashmob Wizard) were instrumental in pioneering the events. The original Philadelphia flashmob spawned others for local sections. If you have interest in organizing a flashmob, please contact either Michelle or Pat. Your COMP Division would be more than happy to help bring this to your neighborhood.

Jeff Evanseck

The **ChemLuminary Awards** began in 1999 as a way of honoring ACS members and volunteers for their efforts on behalf of the Society.

ACS Award for Computers in Chemical & Pharmaceutical Research

Sponsored by Accelrys

Professor Johann Gasteiger of the University of Erlangen-Nürnberg, in Germany is the winner of the 2006 ACS Award for Computers in Chemical and Pharmaceutical Research for his contributions to the field of chemoinformatics.

Gasteiger received a doctorate in organic chemistry from the University of Munich (1971). Following a postdoctoral fellowship at the University of California, Berkeley (1971-72), he taught at the Technical University of Munich. In 1994, he moved to the University of Erlangen-Nürnberg, where he cofounded the Computer Chemie Centrum. He is one of the pioneers of chemoinformatics in Germany and has produced more than 200 scientific publications in this field.

Symposia for Atlanta ACS Meeting

Highlights for Atlanta and preview of the San Francisco ACS Meeting

The Spring 2006 meeting in Atlanta promises to be interesting, as a number of COMP symposium organizers have scheduled a variety of topics ranging from drug discovery to computational methodology.

- Thomas Kuhn Paradigm Shift Award Symposium (*Anthony Nicholls, Geoff Skillman*)
- Protein Kinases: Computer Modeling and Experiment (*Chung Wong*)
- GPCR Structure Modeling and Ligand Design (*John Woolfrey, Irache Visiers*)
- Virtual Screening: Using Structure Based and Ligand Based Methods for Lead Identification (*Lakshmi Narasimhan, Wan Lau, Leslie Kuhn*)
- Frontier Applications and Developments of Density Functional Theory: A Symposium in Honor of Robert G. Parr's 85th Birthday (*Weitao Yang, Paul Ayers*)
- Structure Determination Using NMR and Computational Methods (*J. Phillip Bowen*)
- General Oral – Drug Discovery (*Wendy Cornell*)
- General Oral – Molecular Mechanics and Simulation (*Jeffry Madura*)
- General Oral – Quantum Chemistry (*Jeffry Madura*)

The poster session will take place as usual on Tuesday night. The CCG sponsored Excellence awards will be presented to the students 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. Novartis Institutes for BioMedical Research, Merck Research Laboratories, OpenEye Scientific Software, and Pfizer have all pledged financial support for the Atlanta meeting.

A number of symposia are in place for the Fall 2006 meeting in San Francisco. Please contact Wendy Cornell or Jeffry Madura if you are interested in organizing a symposium. OASYS abstract submission is open through April 25, 2006. Symposia scheduled for the Fall 2006 meeting include:

- Emerging Technologies in Computational Chemistry (*Curt Breneman*)
- Beyond Michael Dewar's Legacy: Modern Semiempirical MO Theory (*Kennie Merz*)
- Molecular Similarity and Indexing Methods (*Ajay Jain, Anthony Nicholls*)
- Tight Binding DFT: Theory and Applications (*John McKelvey*)
- Current Trends in Molecular Docking and Virtual Screening (*Daniel Cheney, Ramy Farid*)
- Structure-Based Design & Development of Estrogen Receptor Modulators (*Veer Shanmugasundaram, Neil Raheja)*
- ADME and Property Prediction (*Daniel McMasters, Matt Walker*)
- General Oral – Drug Discovery (*Wendy Cornell*)

- Careers for Computational Chemists in Pharma, Biotech, Patent Firms, Software and Hardware Vendors, and National Labs (*Wendy Cornell*)
- Free Energy Computations in Drug Discovery (Matthew Clark, Frank Hollinger)
- General Oral – Molecular Mechanics and Simulation (*Jeffry Madura*)
- General Oral – Quantum Chemistry (*Jeffry Madura*)

Thomas Kuhn Paradigm Shift Award

The COMP Division of ACS is pleased to announce a new award symposium -- the "Thomas Kuhn Paradigm Shift Award Competition" -- sponsored by OpenEye Scientific Software. This symposium will take place at the Spring 2006 National Meeting in Atlanta and will focus on talks relevant to drug discovery. Abstracts can be submitted on the OASYS web site (http://oasys.acs.org/) and four will be selected for 40 minute presentations to take place during a half-day symposium at the national meeting. Abstracts not selected for the symposium competition can be moved into the General Oral Drug Discovery symposium (which is always well attended!) if desired.

A panel of judges will select the winning presentation with the speaker awarded a $1000 prize. Talks will be judged on the novelty of viewpoint, the cogency of argument and the potential impact if the speaker's paradigm were to become widely accepted.

About Thomas Kuhn
In the 1940's, while still a graduate student, Thomas Kuhn wrote a monograph on the nature of scientific revolution that was to become the most influential document on the nature of science of the Twentieth Century. Published in 1962 as 'The Structure of Scientific Revolutions', Kuhn described what he saw as the "essential tension" between established ideas, or paradigms, and the new; scientific progress arose by conflict and not consensus. The "Thomas Kuhn Paradigm Shift Award" is designed as an opportunity for speakers to present views at odds with perceived wisdom, with particular emphasis on application to the science of drug discovery.

Chemical Computing Group Excellence Award Recipients Announced

CHEMICAL COMPUTING GROUP
Scalable Software. Scalable Science.

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 subsidize travel expenses to the Atlanta meeting and provide a one-year software license for the CCG Molecular Operating Environment (MOE) (http://www.chemcomp.com/).

The awardees, in alphabetical order, are:

- Xihua Chen: "MFCC-DM with pairwise interaction correction for quantum chemical study of proptein", *New York University*
- Xuhui Huang: "Hydrophobic-Aided Replica Exchange: an efficient algorithm for sampling biological systems in explicit solvent", *Columbia University*
- Casey P. Kelly: "Calculation of acid dissociation constants by the SM6 quantum mechanical implicit solvation model", *University of Minnesota*
- Valerie McCarthey: "Stability of H2 Clathrates vs Cavity Occupancy", *University of Pittsburgh*
- Devina Pillay: "Role of Oxygen Vacancies on Growth of 1B (Au, Ag and Cu) Particles on TiO2(110)", *University of Texas, Austin*

Applications for awards to attend the meeting in San Francisco, CA in September 2006 consist of an extended abstract, CV, personal statement, and a supporting letter from the student's advisor and are **due to Andrew Good by April 11, 2006**. Submissions are restricted to North, Central and South American students. Please see the COMP website for more details.

COMP Division Member Drive

Why Should I Join the COMP division?

COMP members are aware of the many benefits provided by the division, ranging from the Annual Reports in Computational Chemistry (ARCC) to discounts on journals. However, many individuals do not realize the opportunities available to them through membership. We ask our current members to spread the word.

All individuals interested in the use of computers as tools to solve problems in chemistry and related physical and biological sciences are invited to join the COMP Division. Although the primary focus of the Division is theoretical and computational chemistry, the scope of the Division is broad and interdisciplinary.

COMP includes: artificial intelligence, experimental design, and molecular modeling in the fields of agrochemicals, materials science, medicinal and organic chemistry, pharmaceuticals, polymers and theoretical chemistry.

The Division monitors developments in computer hardware, software, and networking and keeps its members informed of new applications in chemistry via symposia and workshops at the National Meetings. The Division promotes undergraduate and graduate student participation and in particular provides travel grants for graduate students to present their work at National Meetings. The COMP division currently has almost 3,000 members.

Benefits of Membership include:

- Career advancement through professional development and networking opportunities
- Opportunity to present papers at National and Divisional Meetings
- Access to abstracts of papers presented at the National Meetings
- Recognition for your contribution to the advancement of chemistry
- Educational and professional opportunities
- Renewed enthusiasm for your professional goals
- Scientific and technical idea exchange that spark new and exciting directions in your work
- Access to the latest trends in areas of special interest
- Input on upcoming symposium topics
- Early notice of upcoming events
- Personal copy of *Annual Reports in Computational Chemistry*
- 30% discount on books from Oxford University Press
- Discount on subscriptions to the *Journal of Molecular Graphics and Modeling*.

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

Join the COMP division!

http://membership.acs.org/C/COMP/

Go to COMP's website to obtain the most complete, up-to-date information available on events, publications and topics within the COMP division.

Journal of Molecular Graphics and Modelling

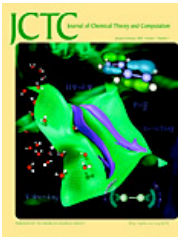
The *Journal of Molecular Graphics and Modelling* (JMGM) has again seen a steady increase in the number of papers submitted and published over previous years. The *Journal* is healthy and widely cited, as indicated by an impact factor (a measure of how many times papers published in the *Journal* are cited in other publications) for 2003 that puts it in the top ***four*** Journals in computational chemistry. It has become a publication venue of choice for many of you and your colleagues. We certainly solicit papers from COMP members and can promise rapid and expert review of your research findings.

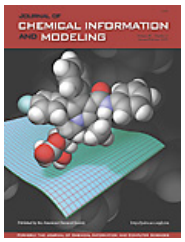
As always, thanks to you and the Editorial Board for your help and support. It's a pleasure to serve as COMP's editor for JMGM.

Andy Holder, U.S. Editor, *JMGM*

JCTC and JCIM

Newest additions to the COMP family





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.

Comp members are encouraged to use JCTC, JCIM and JMGM as a forum for their publications. Articles describing research of substantial merit are invited. For more detailed information on JCTC and JCIM please visit the ACS publications website, http://pubs.acs.org.

Hurricane Relief and Support

ACS Responds to Members Affected by Gulf Coast Hurricanes

Following the devastation to the Gulf Coast wrought by this year's major hurricanes, a Hurricanes Response Task Force was created to identify ways in which the Society can help ACS members who live and work in those areas.

At the recent ACS Board of Directors meeting, the Board voted to accept the recommendations made by the Task Force:

- That the Society declare a suspension of dues for a period of 12 months to the 302 ACS members in the hardest hit regions affected by the Gulf Coast hurricanes. These members will be moved to an unemployed dues waiver status and be treated as "paid active" for a period of 12 months, starting the date following the current paid date.

- That all members (approximately 564) in the postal zip codes that were at one time considered undeliverable be eligible to "opt – in" to the unemployment dues waiver status. Members will have the option to continue their dues as routine, or postpone dues payment via an "opt – in" feature.

The COMP division has followed suit and also suspended divisional dues for our affected members. The Board expressed its appreciation to the Hurricanes Response Task Force for its effective response to this significant crisis.

Upcoming ACS Short Courses

Computational Chemistry, Concepts, Methods, and Practical Approaches, June 5 – 6, 2006, University of North Carolina at Greensboro, Greensboro, NC.

Computer-Assisted Drug Design, Concepts, Methods, and Practical Approaches, June 7 – 9, 2006, University of North Carolina at Greensboro, Greensboro, NC.

Registration for all courses is available on-line. A $500 discounts is available if both classes are taken. More information is available via the COMP website at http://membership.acs.org/C/COMP/.

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