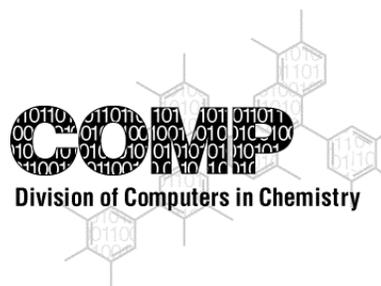


- Award winner to be selected during Emerging Technologies Symposium
- *Journal of Molecular Graphics and Modelling* Editor's report
- Preview of COMP symposia for New Orleans, Spring 2003



COMP Newsletter

Statement from the Chair

Bill Jorgensen, the Chair of COMP, reports on the status of the Division

The ACS national meeting in Orlando was a great success with COMP well represented through nine symposia and the general oral and poster sessions. This included the symposium honoring Tack Kuntz (UCSF) for receipt of the 2002 ACS Award for Computers in Chemical and Pharmaceutical Research. Congratulations go to Tack, and thanks go to Accelrys, Inc. for sponsorship of the award. The poster session also included presentation of the Excellence Awards, sponsored by the Chemical Computing Group, to encourage participation of graduate students in COMP activities.

The Boston ACS meeting (August 18-22) features another set of dynamic COMP symposia, thirteen this time, covering hot topics in quantum chemistry, molecular mechanics, genomics, chemoinformatics, and more. Program Chair and Vice-Chair, Ralph Wheeler and Wendy Cornell, deserve much credit and thanks for continuing the tradition of excellent, state-of-the-art symposia for the COMP division.

The COMP division remains in good financial shape under the watchful eye of Treasurer Curt Breneman, who adheres to a strict no shredding policy. I am happy to report that the dues will be unchanged for

2003, *i.e.*, \$10 for regular ACS members and \$5 for student members. However, we are looking into obtaining on-line access to several key journals in computational chemistry for all COMP members. A dues increase might be considered to help facilitate this. If you have any thoughts on this matter, please email me. Please also check out the COMP website, <http://membership.ACS.org/C/COMP>. Suggestions for changes or additions are most welcome and can be emailed to me or to Lisa Balbes.

Bill Jorgensen

Preview of the Emerging Computational Technologies Symposium

Award will be presented at the Boston ACS national meeting

On Tuesday afternoon, August 20, at the 224th ACS National Meeting in Boston, you are invited to attend the third annual Symposium on Emerging Computational Technologies. The objective of the symposium is to stimulate, reward, and publicize methodological advances in computational chemistry.

At the symposium, the speakers will be competing for the prize of \$1000 generously sponsored again by

Schrodinger, Inc. In addition, free one-year subscriptions to the *Journal of Molecular Graphics and Modelling* will be provided by Elsevier Science. *JMGM* has been affiliated with the COMP Division since 1998.

Over 15 applications to compete in the symposium were received. From these, members of a Panel of Experts selected six scheduled speakers. At the symposium, the talks will be evaluated by the Panel of Experts based on the impact the research will have on the future of computational chemistry and allied sciences.

Hope to see you in Boston!

Donald B. Boyd
Email: boyd@chem.iupui.edu

National Chemistry Week October 20-26, 2002

ACS Career Services Salary Comparator: Estimate salary ranges for (computational) chemists based on specialty, education level, geographic area, and more...

<http://center.acs.org/applications/acscmparator/page01.cfm>

Chemical Computing Group Excellence Award Winners Announced



Chemical Computing Group Excellence
Awards recognize five students

The ACS Division of Computers and Chemistry and the Chemical Computing Group (CCG) presented Excellence Awards to five graduate students in Orlando on April 9th.

In alphabetical order, the winners were:

- **Thomas Dick**, *Duquesne University*: "Computational modeling of brine to aid CO₂ sequestration research"
- **Benoit Leblanc**, *French Petroleum Institute and the Institut National de Recherche en Informatique et Automatique*: "Mixing Monte Carlo moves more efficiently with an evolutionary algorithm"
- **Viera Lukacova**, *North Dakota State University*: "Implementation of multiple binding modes in CoMFA"
- **Sabine Schefzick**, *Indiana University Purdue University-Indianapolis*: "Theoretical ligand distortions in chiral catalysts: Can molecular deformations enhance a catalyst's chirality content?"
- **Xuelin Wang**, *University of North Texas*: "Error analysis in density functional theory: Atomization energies"

The CCG Excellence Awards were created to stimulate graduate student participation in COMP Division symposia and poster sessions at ACS National Meetings. Winners receive a one-year software license of CCG's MOE (Molecular Operating Environment) for their academic research groups, in addition to travel costs. Awardees are chosen on the basis of the quality and significance of the research to be presented and the strength of the supporting materials.

Prior to an ACS National Meeting, an applicant must first follow the steps for OASYS abstract submission by the COMP division deadline. The following materials must then be submitted to the COMP Treasurer:

- 1) An extended abstract of the presentation
- 2) A letter of recommendation from the research advisor
- 3) A personal statement from the applicant

Information on Fall 2002 winners and approaching abstract deadlines (tentatively November 15th) for the CCG Excellence Awards for the Spring 2003 ACS meeting in New Orleans will be posted on the COMP Division web site.

Recent Books by COMP Authors

Michelle M. Francl, [A Survival Guide for Physical Chemistry](#),
<http://www.physicscurriculum.com>

Christopher J. Cramer, [Essentials of Computational Chemistry: Theories and Models](#), Wiley.

Kenny B. Lipkowitz & Donald B. Boyd, [Reviews in Computational Chemistry](#), Vol. 17, Wiley.

COMP Division Web Site News

What's New on the Web?

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

According to ACS's own statistics, COMP's web site is one of the most visited on the membership server. You can now check this out for yourself—there's a counter at the bottom of the home page that tracks the number of visitors. Come yourself and see how popular we are!

Recent additions to the web site include:

- Abstracts from all papers presented at the Spring 2002 meeting in Orlando

- A list of symposia and journal special issues offered this year in memory of Peter Kollman

And as always, the most current newsletter, executive committee meeting minutes, planned programs for upcoming national ACS meetings, and more! Let us know what you'd like to see, and we'll do our best to get it there.

Lisa M. Balbes, WebMaven

225th National ACS Meeting New Orleans, LA, March 23-27, 2003

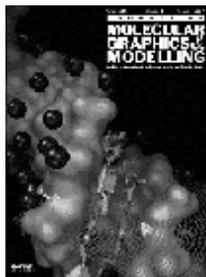
The following symposia are planned for the ACS National Meeting in New Orleans:

- ACS Award for Computers in Chemical and Pharmaceutical Research
- Biological applications of implicit solvent models
- Computational nanotechnology
- Contributions in computational and theoretical chemistry: from the qualitative to the quantitative regimes
- High-throughput computational processes in drug discovery
- Machine learning in computational chemistry
- Multiple length and time scales in molecular modeling
- Protecting your programs—legal issues in computational chemistry
- Protein flexibility
- Recent developments and applications of time-dependent DFT and related *ab initio* and semi-empirical methods
- Small molecule antiangiogenesis discovery
- Teaching medicinal chemistry and drug discovery to undergraduate chemistry majors

For an up-to-date list of symposia for future ACS national meetings, visit <http://www.acs.org> or the COMP division Web site.

Newsletter of the COMP division of the ACS
Fall 2002

Journal of Molecular Graphics and Modelling



U.S. Editor
Andrew Holder
reports on JMGM

JMGM is alive and well! I have completed my first

year as Editor of the *Journal of Molecular Graphics and Modelling*, representing the ACS COMP division. Since taking over in May 2001, I have received 51 manuscripts. Many of these papers are from COMP members, and *JMGM* is becoming a preferred venue of publication for several important areas of computational chemistry. An important part of *JMGM's* continued success is the mutually beneficial association with the COMP Division. The COMP membership receives a number of clear benefits from the association:

- COMP members get a MUCH reduced rate for both paper and electronic subscriptions.
- The COMP Executive Committee has direct access to me and can help shape editorial practices and procedures. This improves the publication environment for all members.
- Special issues are often produced describing the excellent scientific work that COMP members present at the ACS National Meetings. (Two are in process now.)

A number of changes have been implemented over the past year. First, Jonathan Essex (University of Southampton, UK) has replaced Ron Hubbard as the Editor representing the Molecular Graphics and Modelling Society (MGMS). We have already established a close relationship and things are progressing well on cooperative issues. Second, the first papers in our new Programs section have been published. This section highlights new software available to the *JMGM* community; programs will be downloadable from the MGMS web page (<http://www.mgms.org/>).

Third, given sufficient papers, the publisher, Elsevier, is willing to increase the annual page budget. This will result in a more open and accessible publication outlet for COMP members. Fourth, we have greatly reduced publication delays and are usually able to get a paper through the publication process in less than two months. Fifth, we will soon offer fully electronic submission of manuscripts through COMP's web page. No more mailing huge packets! The future offers still more opportunities for advancing our collaboration, so stay tuned.

Lastly, send me papers!

Andy Holder

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