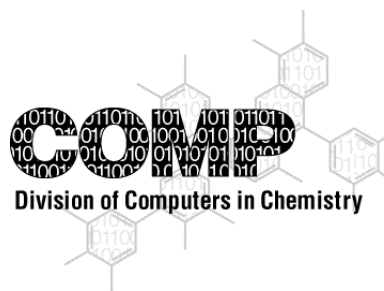


- Chemical Computing Group Excellence Awards
- C&E News features COMP Symposium
- COMP Journal: Journal of Molecular Graphics and Modelling



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# COMP Newsletter

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## eStatement from the Chair

*David Spellmeyer, Chair of COMP, reviews the status of the Division and highlights several new COMP initiatives*

I am pleased to be able to tell you that at mid-year 2001, the COMP division is in very good shape. We are financially sound, have an increasing membership base, and have just completed a successful Technical Program at the Spring National Meeting.

In our last newsletter, we described our successful long-range planning sessions held at Stone Mountain Retreat. Several ideas and initiatives from this meeting have been put in place and some are already showing benefit to the Division. Here are a few:

- Pharmacopeia has agreed to fund the *ACS Award for Computers in Chemical and Pharmaceutical Research* (pending approval by the ACS Board of Directors) under its Software Subsidiary's new name, Accelrys. This substantial investment in the Computers in Chemistry Division is very much appreciated! Peter Gund deserves a great big Thank You from the Division for his role in obtaining this funding.
- We have a permanent Public Relations Chair, a position appointed by the Chair. Shawn Kenner has agreed to take over as our Public Relations Chair for an 18-month term. In this new

role, Shawn will be responsible for coordinating our efforts in publicizing the Division.

- Our website continues to be a major point of focus. Thanks go to Lisa Balbes as she continues to upgrade the COMP Division website, found at <http://membership.acs.org/C/COMP/>
- We have focused on increasing our membership base. At the San Diego ACS meeting, we handed out leaflets describing the benefits of COMP membership. You will continue to see these sorts of outreach efforts expanded.
- We have increased our focus on Multidivisional Programming. You will continue to see an emphasis on cross-divisional programming in the coming years.
- Wendy Cornell has joined the Executive Committee as Assistant Program Chair. Wendy will work with Ralph Wheeler to continue our expansion of COMP National programming.
- We have agreed to fund travel for academic members of the COMP executive team. This should increase our ability to recruit academic members of the COMP team.
- We have initiated a process to amend our by-laws to allow for a two-year term for the Chair. Currently, our Chair serves one year each as Chair-Elect, as Chair, and as Past Chair. Feedback from Divisional Leaders

consistently reflects the desire to increase the one-year term as Chair to allow for continuity in Divisional Leadership. You can expect to see a by-laws change in the next few months.

I'm looking forward to seeing more results from our first long-range planning meeting. The meeting was such a success that we plan to meet as a group again this summer in Las Vegas. Topics will include increasing membership value, the by-laws changes needed for the Chair term, and a structure for volunteering. You will see a report on the results of this meeting in our next newsletter.

### JMGM

Several changes are happening with the Journal of Molecular Graphics and Modeling. After a successful 3-year tenure, Don Boyd will be stepping down as North American Editor. Don has turned around the JMGM during his tenure. Less than 10 papers were submitted in 1998, and over 90 submitted in 2000. A heartfelt Thank You to Don for his service. Andy Holder (whose term as Division Secretary finishes this year) has agreed to be North American Editor of JMGM. Congratulations to Andy on his new position. The publication itself will also be undergoing changes. Elsevier Science has proposed some format changes that will make the journal more readable and more profitable. You will see these changes sometime in 2002.

## Student Excellence Awards

The Chemical Computing Group continues to fund the Student Excellence Awards, which are merit-based awards for graduate students that provide funding to attend National meetings and personal licenses for the MOE software. The second set of Awards was handed out at the 2001 ACS Spring Meeting in San Diego.

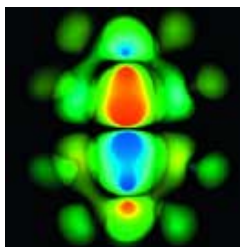
## Officer Training and Planning Meetings

Bill Jorgensen, Curt Breneman, and I attended the Divisional Leaders Training session held in Galveston, TX, in February 2001. The training session was positive for all of us. We spent time discussing membership and volunteer growth, possible new symposia, and divisional structure. We will expand on these issues at our Divisional Long-Range Planning session in June.

The Division Officers continue to solicit input from current and potential COMP Members and to use your suggestions to improve the benefits of Division Membership. If you have ideas about how to improve the Division, about potential Symposia, or would like to volunteer to participate, please contact any of us. Our names and addresses are found later in this newsletter.

David Spellmeyer

## COMP Symposium Featured in C&E News Cover Story



*"Chemists emerge as major players in developing tools for new computer architectures, including increasingly*

*popular computer clusters"*

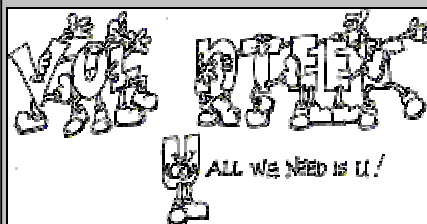
C&E News, April 30, 2001

A symposium sponsored by COMP at the San Diego meeting was selected as the cover story for the April 30, 2001 issue of

C&E News. The symposium, New Computer Architectures in Chemistry-Challenges and Benefits was organized by Andy Pineda of the Albuquerque High Performance Computing Center and featured papers on novel computer architectures, the performance of parallelized computational chemistry software on these new architectures, and new methods in data visualization.

Read the C&E News report at <http://pubs.acs.org/cen/coverstory/7918/7918supercomputer.html>

## Are you COMP's next Newsletter Editor?



As Newsletter Editor you will compile contributions for the twice-yearly publications of the Division Newsletter and interact with other members of the COMP Executive Committee on a wide variety of topics.

If you've been thinking about getting involved in division leadership, consider working on the newsletter—it's a great place to start.

If you are interested I'd be pleased to tell you more about it. Please contact me at [shawn@spotfire.com](mailto:shawn@spotfire.com) 617 702 1522

Shawn Kenner



## Winners of the Chemical Computing Group Excellence Award Announced

*Chemical Computing Group Excellence Awards awarded to three students*

Three students have been recognized as the recipients of the second round of Chemical Computing Group Excellence Awards. Through this program, the Chemical Computing Group provides COMP with \$11,500 annually to fund merit-based student travel awards. The awards defray student travel expenses for ACS national meetings. In addition, CCG provides each of the recipients a \$2,000 one-year license of their Molecular Operating Environment (MOE) software, to be used by their academic institution for research. MOE is used by chemical researchers in the pharmaceutical and biotechnology fields.

Awardees are:

**Gregory W. Kauffman** for the paper entitled "Quantitative Structure-Activity Relationship Models for the Prediction of Selective Cyclooxygenase-2 Inhibition" Co-author of the paper is Peter C. Jurs. Mr. Kauffman is a graduate student in Peter Jurs' labs in the Department of Chemistry, Pennsylvania State University, University Park, PA.

**Larry O. Lockwood, Jr.** for the paper entitled "Comparison of Genetic Algorithm-Based Descriptor Selection Methods for QSAR". Co-authors of the paper are Mark J. Embrechts, Curt M. Breneman, and Kristin P. Bennett. Mr. Lockwood is a graduate student in Curt Breneman's labs in the Department of Chemistry, Rensselaer Polytechnic Institute, Troy, NY.

**C. Matthew Sundling** for his paper entitled "Advances in Electronic Property-encoded Molecular Shape Descriptors" Co-author of the paper is Curt M. Breneman. Mr. Sundling is a graduate student in Curt Breneman's labs in the Department of Chemistry, Rensselaer Polytechnic Institute, Troy, NY.

Award winners are selected from the pool of students submitting poster abstracts to the COMP program. For further information on the Chemical Computing Group Excellence Awards program, including how to submit an abstract to the competition, see the COMP Division web site <http://membership.acs.org/C/COMP/>. For more on MOE and CCG see <http://www.chemcomp.com>.

Fall 2001 winners will be announced in the Spring 2002 COMP Newsletter.

## Secretary's Report

*COMP membership grows by 13%*

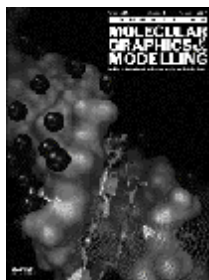
Membership in the Division increased from 2355 at the end of 1999 to 2668 at the end of 2000. This represents a 13.3% increase in one year, and is a strong positive result of ACS's Member Get a Member emphasis. COMP membership grew more than almost any other Division over the same period.

By the time you read this elections will have been completed for our new officers for 2002. Check the website for results.

By unanimous consent, the Executive Committee extended the term of Treasurer Curt Breneman by one year to end in 2002. In this way, terms for the Secretary and Treasurer will not expire in the same year, providing better continuity among the officers.

Andy Holder

## JMGM: The Division's Own Journal



*JMGM changes editorship: Don Boyd passes the reins to Andy Holder*

As many of you are aware, Don Boyd stepped down in April after a VERY distinguished term as Editor of the *Journal of Molecular Graphics and Modelling*. Don is credited with virtually resurrecting the journal during his time as editor. At the

Executive Committee Meeting in San Diego, the Committee gave Don an enthusiastic and well-deserved round of applause for his excellent work. Thank him for his efforts both for the Division and JMGM when you see him!

I have accepted the position of Editor at JMGM and look forward to continuing the growth of the journal. Many of you may not realize the closeness of the ties between JMGM and our Division. First, COMP members get substantial discounts on personal subscriptions. Second, the Editor attends Executive Committee Meetings and reports the goings-on at the *Journal*, and the EC has an opportunity to make suggestions and contributions. Third, COMP appoints the US Editor in cooperation with Elsevier Science. So, the COMP EC has direct involvement with the editorial practices and procedures of a journal specializing in the Division members' area of interest. The involvement leads to a better and more focused publication in our field. Both the COMP Division and Elsevier benefit from the relationship.

Don was successful largely due to the cooperation between our Division and the *Journal*. A number of special issues were produced during his time at the helm and more are planned in connection with COMP symposia at national meetings. While these are important, the backbone of any journal is the stream of submitted papers. I encourage you to send me papers, and I commit to timely, efficient, and fair review and publication of your submissions. We are willing to accept papers from almost any sub-discipline of computational chemistry in our desire to make JMGM a premier scientific publication with which the COMP Division of the ACS will be pleased and proud to be associated.

Andy Holder

[**Editor's note:** For more information on JMGM, including reduced subscription rates for COMP members please see the COMP web page: <http://membership.acs.org/C/COMP/>]

**223rd National ACS Meeting  
Chicago, IL, August 26-30, 2001**

*COMP has been identified as one of six areas of concentrated programming for the 223rd National ACS Meeting in Chicago. COMP will sponsor symposia in thirteen areas at the spring show.*

Planned COMP symposia include (co-sponsoring divisions listed):

- 1) Cheminformatics (CINF, MEDI)
- 2) Computational Organometallic Chemistry (INORG)
- 3) Docking and Testing
- 4) Emerging Technologies
- 5) Linking Genomic Information with Drug Design (CINF, MEDI)
- 6) Modeling Ligand Interactions with Membrane Proteins
- 7) QM/MM Methods (PHYS)
- 8) Computational Chemistry in the Undergraduate Curriculum (PHYS)
- 9) Computational Modeling and Simulation of Self-Assembled Materials (COLL)
- 10) Computer Modeling of Polymers (PMSE)
- 11) First Principles Simulations of Chemical Dynamics (PHYS)
- 12) Information Challenges in CombiChem/HTS Era (CINF)
- 13) Using Computers to Teach Biochemistry (CHED)

For an up-to-date list of symposia for future ACS national meetings, visit <http://www.acs.org>. At press time, tentative topics for symposia at future national meetings include:

### Orlando, Spring 2002

- 1) Ab initio Molecular Dynamics
- 2) Carbohydrate Modeling
- 3) Chemometrics
- 4) Enhanced Sampling Techniques in Molecular Dynamics and Monte Carlo Simulations
- 5) Modeling Nucleic Acids
- 6) Molecular Modeling Across the Periodic Table

- 7) Molecular Modeling and the Experimental Validation of Reaction Mechanisms
- 8) QSAR
- 9) Rational Drug Design
- 10) Recent Advances in Electron Correlation Methodology

#### Boston, Fall 2002

- 1) Emerging Technologies
- 2) New Developments in Force Fields for Molecular Modeling
- 3) Semi-empirical Molecular Orbital Methods
- 4) Computational Chemistry in Chemical Education
- 5) Classical and Quantum Statistical Mechanics Studies of Solvation
- 6) QSAR
- 7) Linking Genomic Information with Drug Design?
- 8) Conformational Analysis
- 9) Chemistry of Computers

#### COMP Division Web Site Continues to Improve

The COMP division web site at <http://membership.acs.org/C/COMP/> continues to grow. Current information on programming for future meetings is always available. In addition, we have added complete COMP division program information for past ACS national meetings, all the way back to 1998. Minutes of the Executive Committee meeting for the March 2001 meeting are now available. More historical information is added as it becomes available.

Let me know what else you would like to see on the web site, and we'll do our best to get it there.

Lisa M. Balbes, WebMaven

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#### COMP Web Site Archives Historical Information

*Building a COMP Archive starts with the past!*

We've heard from the membership that you want more historical information on the web site - officer listings from past years, back issues of the newsletter, past national meeting programming, and so on. In order to put this information on-line, we first have to find it! I've gotten everything available from the national office, now I'm appealing to the membership.

If you were an officer, chaired a session at a national meeting, etc. and still have the details, please send the information to me, so we can fill in our archives.

Lisa Balbes [lisa@balbes.com](mailto:lisa@balbes.com)

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