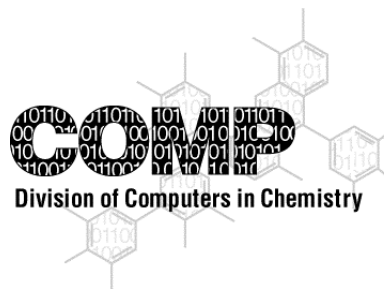


Spring 2002 Highlights

- New COMP Division Officers Begin Service
- Irwin D. Kuntz to be Honored with ACS Award for Computers in Chemical & Pharmaceutical Research
- Abstract Deadlines Approaching for the Emerging Technologies Symposium and CCG Excellence Awards



COMP Newsletter

Statement from the Chair

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

It has been a pleasure to become closely involved with the COMP division during the last year. The division is a truly vibrant one that has been nicely growing over the last three years to a total membership of about 3000, which places us in the top half of ACS divisions by size. The growth reflects the ever increasing interest in and importance of computational chemistry. It also reflects the great effort and enthusiasm of the COMP division's members and officials in promoting and participating in the division's wide-ranging activities, especially the dynamic symposia at ACS meetings. Program Chair Ralph Wheeler, Vice-Chair Wendy Cornell, Webmaster Lisa Balbes, and newsletter editors Shawn Kenner and Michelle Lamb deserve special thanks for making the innumerable arrangements and keeping us informed. I also want to publicly thank our treasurer, Curt Breneman, for the extreme effort required to understand and repair the Division's tax situation. We are in good shape both spiritually and financially. I also welcome the newly elected officers (see below); their willingness to serve is much appreciated by us all.

It would be nice not to close on a sad note, but it is impossible not to mention the loss of Peter Kollman last May. Peter was a central figure in the COMP community, a mentor to many, and friend to all. There will be a memorial COMP symposium at the Orlando ACS meeting on Monday April 8, 2002. There are also special issues *Biopolymers* (contact Ken Dill, dill@maxwell.ucsf.edu) and *the Journal of Computational Chemistry* (contact me) that will be dedicated to Peter. Your attendance at the symposium and contributions to the journals are most welcome.

Bill Jorgensen

Statement from the Past Chair

David Spellmeyer reviews his year as Chair

This past year has been a very exciting year for the Computers in Chemistry Division of the American Chemical Society. I consider it a privilege to have served during this exciting year. We have made many advances, including a rather substantial increase in membership, a renewed relationship with the Journal of Molecular Graphics and Modeling, and continued excellent programming at National Meetings. We have also redefined the role

of the Chair-Elect and Past Chair to provide more continuity on long-term projects.

None of this work could have been accomplished without a dedicated group of volunteers. It has been a pleasure to work with the Executive Committee during the past two years and I look forward to my remaining year on the Committee as Bill Jorgensen takes over the helm as the Division's Chair.

Words are insufficient to convey my deep gratitude to the individuals who volunteer their time to make this Division work and to continue to improve the value of COMP membership. I would like to extend my special thanks to Joyce Kostura, my former assistant, who ensured that I missed no deadlines with the ACS, arranged the Executive Committee summer planning retreat, booked much travel, and compiled our membership flyer. I am indebted to her.

I also thank each of you who, as members, continue to support the COMP Division. I am sure that you will continue to see your membership value grow during the coming years.

David Spellmeyer

Report from the Division Secretary

Newsletter of the COMP division of the ACS
Spring 2002

2001 COMP Division Election Results

Our election is over and the results are as follows for your new 2002 Officers. Congratulations! Members take a moment to thank these folks for their time and service.

Chair-Elect: Peter Grootenhuis

Secretary: Jeff Evanseck

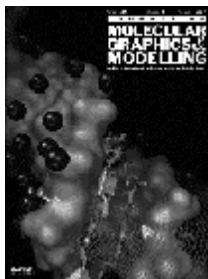
Councilor: Michelle Francil

Alternate Councilor: Hanneke Jansen

As noted above, by the time you read this, Jeff Evanseck will be the Division's new Secretary. Good luck, Jeff! I have enjoyed serving the Division and I thank all of the members for their support over the past three years.

Andy Holder

The Division's Own Journal



Editor Andrew Holder reports on JMGM

I have been North American Editor of the *Journal of Molecular Graphics and Modelling* (JMGM) since May, and it has been an exciting and educational time. A number of articles have come in over the last few months, and the Journal continues to strengthen. There will be nine issues published this year instead of the normal six to clear out the backlog of papers that had built up. We are now back on schedule and are able to process submissions at a reasonable rate for quick publication.

Several special issues are planned dealing with COMP symposia, so be on the lookout for those. In support of the Emerging Technologies Symposium conducted in Chicago in the Spring of 2001, free one-year subscriptions to JMGM were provided for all presenters.

The COMP Executive Committee has extended our relationship with JMGM for

another two years. I encourage members of the Division to consider publishing in JMGM. I will continue to attend Executive Board meetings as JMGM's representative. I want to hear from you about what you think would improve the Journal and its service to the membership.

Andy Holder

Chemical Computing Group Excellence Award Winners Announced



Chemical Computing Group Excellence Awards awarded to five students

In Chicago, five students received Excellence Awards sponsored by the Chemical Computing Group, Inc. (<http://www.chemcomp.com/>). Award winners were selected from the pool of students submitting poster abstracts to the COMP program. The winning students, who received a certificate, a one-year license of the CCG Molecular Operating Environment software, and travel reimbursement, were:

- Caterina Bissantz, ETH, Zurich, Switzerland: Virtual Screening of Chemical Databases: Application of G-protein Coupled Receptors
- Catherine Check, Northern Illinois University: Augmentation of the LANL2DZ Basis Set under B3LYP and MP2 Models to Improve Calculated Results for p-Block Elements
- Norge Cruz Hernandez, Seville University, Seville, Spain: DFT and Molecular Dynamic Study of the ScN, TiN and VN Materials
- Ohyun Kwon, Auburn University: Theoretical Studies of Main Group Metalloenes

- Nelaine Mora-Diez, Dalhousie University, Nova Scotia, Canada: Theoretical Calculations in Atmospheric Chemistry: OH and NO₃ Hydrogen-Abstraction Reactions from Aldehydes

Information on Spring 2002 winners and approaching abstract deadlines for the CCG Excellence Awards for the Fall ACS meeting will be available on the COMP Division web site.

Winning Paper at the Emerging Technology Symposium

Award presented at the Chicago, IL ACS national meeting

The second annual Symposium on Emerging Computational Technologies was held at the 222nd American Chemical Society National Meeting, Chicago, Illinois, August 28, 2001. This COMP symposium was held as part of the celebrations of the 125th anniversary of the American Chemical Society.

Each year, the objective of the symposium is to stimulate, reward, and publicize methodological advances in computational chemistry. The talks are evaluated based on the impact the research will have on the future of computational chemistry and allied sciences.

The symposium was sponsored by [Schrodinger, Inc.](#), which provided the \$1000 prize to the winning speaker, Dr. Christopher E. Keefer, of GlaxoSmithKline. An excellent report of this symposium, by Elizabeth K. Wilson, appeared in the October 8, 2001 issue of *Chemical & Engineering News*.

Irwin D. "Tack" Kuntz to be Honored

2002 ACS Award for Computers in Chemical & Pharmaceutical Research, sponsored by Accelrys, Inc.

On April 9, Irwin D. Tack Kuntz, of the Department of Pharmaceutical Chemistry of University of California, San Francisco, will be honored with the ACS Award for Computers in Chemical and Pharmaceutical Research. Professor Kuntz is the director of the Molecular Design Institute and Associate Dean of Research in the UCSF School of Pharmacy.

While he has varied research interests in biophysics, physical chemistry, and NMR spectroscopy, Kuntz may be best known for his work on molecular docking and its application to drug design. The widely used program, DOCK, was developed in his laboratory at UCSF.

The award, given annually and sponsored by Accelrys Inc., recognizes outstanding contributions to the advancement of the use of computers in the chemical and biological sciences.

**223rd National ACS Meeting
Orlando, FL, April 7-11, 2002**

Chemistry and Computers has been identified as an area of concentrated programming for the 223rd National ACS Meeting in Orlando, FL.

COMP Planned Program:

- ACS Award for Computers in Chemical & Pharmaceutical Research
- ACS COMP Division Symposium in Remembrance of Peter A. Kollman
- Carbohydrate Modeling
- Enhanced Sampling Techniques in Molecular Dynamics and Monte Carlo Simulations
- Modeling Nucleic Acids
- Molecular Modeling Across the Periodic Table
- Near-Neighbor Searching for Lead Follow-up: Algorithms and Descriptors
- Rational Drug Design

- Recent Advances in Electron Correlation Methodology
- Tools for Exploring Potential Energy Surfaces for Chemical Reactions

Related Symposia:

- Making Effective Use of the Virtual Classroom (CHED)
- ADME/Tox Informatics (CINF)
- Chemical Descriptors (CINF)
- New Developments in Electronic Publishing (CINF)
- Polymer Informatics (CINF)
- Standards for Chemical Informatics (CINF)
- Visualization of Chemical Information (CINF)
- Computational Methods in Fuel Science (FUEL, PETR)
- Frontiers in Chemical Dynamics (PHYS)
- Molecular Modeling & Simulation of Reaction Mechanisms, Kinetics & Catalysis (PHYS)

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

COMP Division Web Site News

New Additions to the Division's Web Site

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

The COMP division web site continues to be regularly updated — the most up to date information is always available there. In fact, this newsletter will be available on-line before you get it in postal mail! Details on all the following activities can now be found on-line:

About you:

- Demographic Data describing COMP division members

Officer activities:

- Minutes from the Executive committee meeting at the Fall national meeting

- Results of the election for COMP division officers
- Complete list of officers and their contact information for 2002

Program listings:

- Complete technical program and abstracts from the Chicago national ACS meeting
- A guide for symposium organizers, updated Fall 2001

Moneysaving offers:

- A discount on Reviews in Computational Chemistry is now available for division members

Awards:

- Winners of the CCG Excellence Awards and Emerging Computational Technologies symposium prize
- Detailed information and abstract submission deadlines for upcoming awards

Check the web site regularly for updated information. If you have material to contribute, or ideas for other information that should be there, please let me know.

Lisa M. Balbes, WebMaven

Abstracts Due for the Third Annual Symposium on Emerging Technologies

\$1000 prize to be given at the Boston ACS national meeting, August 2002

The Computers in Chemistry Division (COMP) will be holding the *third* annual Symposium on Emerging Technologies at the American Chemical Society National Meeting, Boston, Massachusetts, August 18-22, 2002.

To participate, it is necessary to submit a regular short ACS abstract via <http://oasys.acs.org/>. It is also necessary that a long (1000-word, text-only) abstract be e-mailed to the organizer no later than April 9, 2002.

The talks must be original and not be repeats of talks at other ACS symposia. The long abstracts will be evaluated, and those individuals selected for an oral presentation at the symposium will be notified by the end of April. Applications for the Symposium that cannot be accepted will be rescheduled into one of the other COMP sessions.

The long abstract and inquiries should e-mailed to the organizer of the symposium:

Prof. Donald B. Boyd,
Editor, [Reviews in Computational Chemistry](#)
Department of Chemistry
Indiana University-Purdue University at Indianapolis (IUPUI)
Indianapolis, IN 46202-3274, U.S.A.

Email: boyd@chem.iupui.edu

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