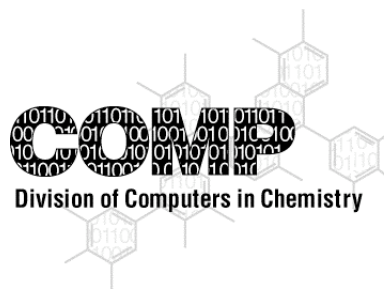


Spring 2003 Highlights

- Ten Students to Receive CCG Excellence Awards in New Orleans
- Ken Houk to be Honored with ACS Award for Computers in Chemical & Pharmaceutical Research
- M. J. S. Dewar Symposium Endowed, to be Held in Spring 2004



COMP Newsletter

Statement from the Chair

Peter Grootenhuus will lead the Division in 2003

Following a person that is so widely known in the chemistry community as Bill Jorgensen is never easy, so please allow me to briefly introduce myself. My name is Peter Grootenhuus, and I am currently employed at Vertex Pharmaceuticals in San Diego, where I carry responsibility for the computational chemistry and lead discovery efforts. Before I came to the USA in 1998 to join Combichem, Inc., I worked and lived in the Netherlands.

Becoming closely involved with the COMP Division has been a truly rewarding experience for me during my year as Chair-Elect: the people are great, and the science is great. Historically, the COMP Division has been very active in organizing high quality symposia and activities. As always, this year a number of exciting symposia will be organized. In 2003, we will continue to expand our services for COMP Division members. We are in the process of evaluating whether we can produce an annual update of relevant computational chemistry trends and developments somewhat related to the highly successful *Annual Reports in Medicinal Chemistry* publication of our sister Medicinal Chemistry Division (MEDI). We see this as a great opportunity to get more scientists interested in Computational Chemistry and

perhaps further grow the membership of the COMP Division.

On behalf of the COMP Division members, I would like to thank Bill Jorgensen for being an outstanding Chairman. We look forward to his continued involvement as Past-Chair. Other changes within the Executive Committee include the departure of Tamara Gund (Alternate Councilor, 2000-2002) and plans for David Spellmeyer (Past Chair, 2002) to pursue the abovementioned annual computational update. Following last summer's elections, we welcome Michelle Francl, Chair-Elect for 2003 (and continuing Councilor, 2002-2004), and Jennifer Miller, Councilor (2003-2005) into new leadership roles within the Division.

I look forward to serving you this year as Chair and hopefully will meet you at one of the many COMP symposia in New Orleans or New York.

Peter Grootenhuus

Statement from the Past Chair

Reflections on COMP Division activities in 2002

It was a pleasure to serve as Chair of the COMP Division during the last year. The division remains in good shape in all areas. All aspects of the programming, especially

the quality, quantity, and attendance, for the National Meetings remain truly impressive owing to the efforts of the COMP membership and leadership of the Program Chair, Ralph Wheeler, and Vice-Chair, Wendy Cornell. The COMP website and newsletter have also evolved nicely under the guidance of Lisa Balbes and Michelle Lamb. Special recognition goes to Curt Breneman for keeping us well-guided financially and for administering the Chemical Computing Group awards, and to Jeff Evanseck for myriad form-filing efforts and running the annual elections. Of course, special thanks go to Chemical Computing Group including Pam Newton and Paul Labute for their generous sponsorship of the CCG awards and to Accelrys including Scott Kahn and Peter Gund for their generous sponsorship of the ACS Award for Computers in Chemical and Pharmaceutical Research, which will be extended to Prof. Ken Houk at UCLA this year.

In July, Erin Duffy and I had the pleasure of hosting the annual Executive Retreat for the COMP Division in New Haven. Many issues were discussed, including closer ties with other ACS divisions and further enhancements to COMP-membership value through possible production of an *Annual Reports in Computational Chemistry* and electronic journal access for COMP members. You will hear more on these topics during the coming year, and your input on all COMP matters is always

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welcome—the committee members' contact information can be found at the end of this newsletter. I now turn over the Chairmanship to Peter Grootenhuis with full confidence in the future of COMP.

Bill Jorgensen

Letter from the Program Chair

Highlights in New Orleans and upcoming symposia

Through the efforts of many dedicated hard-working people, the COMP Division's technical programming at national meetings continues to expand and improve. As in 2001, Chemical & Engineering News chose to highlight two of our symposia with cover stories in 2002. The April 29 issue featured an ADME/Tox symposium co-sponsored by the COMP Division and the September 16 cover featured our symposium on Computational Chemistry in Chemical Education, organized by Theresa Zielinski (co-sponsored by CHED). The number of presentations has more than doubled since 2000 and in New Orleans, we anticipate a record 386 technical presentations(!), plus numerous talks in symposia co-sponsored with other divisions.

The program for New Orleans includes the presentation of the ACS Award for Computers in Chemical and Pharmaceutical Research to Ken Houk on Tuesday afternoon. In addition, the poster session, with more than 100 posters, will be held Tuesday evening. The presentation of CCG Excellence Awards to ten outstanding graduate students will also occur at that time. I hope you will come to the poster session, enjoy the refreshments and the science (**new 6 pm start time--don't be late!**), and ask tomorrow's leading computational chemists about their work.

A number of visionary individuals and generous organizations are also working to make the future of COMP programming look especially bright. Not only has the Chemical Computing Group doubled the number of CCG Excellence Awards, but also Accelrys is supporting the ACS Award for Chemical and Pharmaceutical Research,

and Schroedinger Inc. has agreed to continue support of our annual "Emerging Technologies" symposium. A special thanks is due to Don Boyd for his work to establish and organize the first three Emerging Technologies symposia.

In 2004, we expect to hold the first of several symposia sponsored by Elsevier (arranged by Andy Holder) and the COMP Division's first endowed symposium in honor of an eminent chemist, M.J.S. Dewar, will be held in the Spring. The annual Dewar Symposium will be devoted to varying topics and is supported by seed funding from Semichem Inc. Additional donations will be gratefully accepted. The symposium was initiated through the vision and generosity of Semichem's founder and President, Andy Holder.

Ultimately, the success of our national meetings depends upon member participation. So please tell graduate students planning to present their work in the COMP Division's program in New York next Fall that the CCG Excellence Awards will pay travel expenses to the meeting and provide a one-year license for the CCG software package MOE. Applications consisting of an extended abstract, vitae, personal statement, and a supporting letter from the student's advisor are due to Curt Breneman before April 14, 2003. Also, anyone wishing to compete for the \$1000 cash prize given for the best presentation in the Emerging Technologies symposium should take time out from preparing his/her tax return to submit an extended abstract to Curt Breneman before April 14, 2003.

If you would like to see a symposium on your favorite topic at a future national meeting, contact me or Wendy Cornell to volunteer or suggest an appropriate organizer. The quality of our programs at national meetings depends on you. So I look forward to hearing from you and learning about your science as we work together to ensure that COMP programming continuously evolves to serve your changing needs.

Ralph Wheeler

Chemical Computing Group Excellence Award Winners Announced



Chemical Computing Group Excellence Awards will be awarded to 10 students

In New Orleans, the following students will receive Excellence Awards sponsored by the Chemical Computing Group, Inc. (<http://www.chemcomp.com/>). Awardees were selected from the pool of students submitting abstracts to the COMP program. Winning students will present their work at the Division poster session, and each will receive a certificate, a one-year license of the CCG Molecular Operating Environment software, and up to \$1,150 reimbursement of travel expenses. Chemical Computing Group, sponsor of awards to five students at each of the past five ACS National Meetings, generously increased their support for this and future meetings so that 10 students may be recognized for their achievements.

- Ivaylo N. Ivanov, University of Pennsylvania: "Relative pKs from First Principles Molecular Dynamics: The Case of Histidine Deprotonation"
- Bethany Kormos, University of Minnesota: "Utilizing Density Functional Theory to Study Nucleophilic Substitution Reactions: Optimization of an Adiabatic Connection Method and its Application"
- Christine Aikens, Iowa State University: "Molecular Electronic Structure and Magnetic Properties of $Y_2Ti(\square-X)_2TiY_2$ (X, Y=H, F, Cl, Br) Isomers"
- Haitao Dong, University of Oklahoma: "Quasiharmonic Vibrations of Water, Water Clusters, and Liquid Water from Principal Component Analysis of Quantum or QM/MM Trajectories"

- Guanglei Cui, SUNY, Stony Brook: "The Complicated Folding of a Simple Peptide Studied by Multiple Folding Simulations and Replica Exchange Approach"
- William B. Katt, Rensselaer Polytechnic Institute: "Optimization of Molecular Properties Through Structural Mutation and Virtual Screening with QSAR Models"
- Zhigang Zhou, Duquesne University: "Resistant Effect Exploring of HIV-1 RT Mutation by Molecular Dynamics"
- Bentley Strockbine, SUNY, Stony Brook: "Advances in Structure Prediction Techniques"
- Min Wu, New York University: "Structural Studies of an Environmental Carcinogen within a Y Family Bypass DNA Polymerase"
- Nicolae-Viorel Buchete, Boston University: "The Effect of Relative Side Chain Orientations on the Ability of Statistical Potentials to Identify Native-Like Structures of Proteins"

Details including each student's graduate advisor and abstract submission procedures of the CCG Excellence Awards for the Fall 2003 ACS meeting are available on the COMP Division web site. The deadline for applications for the New York meeting is April 14, 2003.

ACS Award for Computers in Chemical & Pharmaceutical Research

Professor Ken Houk to be honored in New Orleans

On Tuesday afternoon, March 25th, Professor K. N. Houk, Professor of Organic and Theoretical Chemistry in the Department of Chemistry and Biochemistry at UCLA, will receive the ACS Award for Computers in Chemical and Pharmaceutical Research at a symposium in New Orleans. 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.

Ken Houk received his undergraduate and graduate degrees at Harvard, working with Professor R. B. Woodward as a graduate student in the area of experimental tests of orbital symmetry selection rules. He started at Louisiana State University in Baton Rouge, rising through the ranks to the rank of Professor. In 1980, he moved to the University of Pittsburgh where his involvement in computational chemistry was accelerated through the influence of Kenneth Jordan and John Pople at Carnegie Mellon University. In 1986, Houk joined the faculty at UCLA.

Professor Houk is an authority on theoretical and computational organic chemistry, and his group is involved in developments of theories to understand reactivity, the computer modeling of organic and biochemical reactions, and experimental tests of the predictions of theory. He has published over 500 articles in refereed journals and is one of the top 100 cited chemists of the last two decades. Recently, he was elected to the American Academy of Arts and Sciences.

News from the Emerging Technology Symposium

Third annual symposium held in Boston, August 20, 2002

This symposium was organized by Professor Donald B. Boyd, Indiana University- Purdue University at Indianapolis, under the auspices of the ACS COMP Division to stimulate, reward, and publicize significant methodological advances in computational chemistry.

Interest in the symposium was especially high last year, with a record number of applications being received and a record number of attendees (140) coming to hear the talks and ask questions of the six speakers.

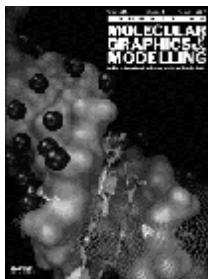
The six contestants included:

- Prof. Vitaly A. Rassolov, University of South Carolina: "Geminals-based Model Chemistry"
- Prof. GaunHua Chen, University of Hong Kong: "Linear-scaling Quantum Chemistry Method for Ground and Excited States: Localized-Density-Matrix Method"
- Mr. Nitin Rathore, University of Wisconsin-Madison: "Monte Carlo Simulation of Proteins through a Random Walk in Energy Space"
- Ms. Chia-En Chang, University of Maryland: "Direct Calculation of Molecular Free Energies"
- Dr. Tudor I. Oprea, formerly at AstraZeneca, now at the University of New Mexico School of Medicine: "High Throughput Prediction of Passive ADME Properties from Fragments"
- Dr. Christophe Cleva, Serono Pharmaceutical Research Institute, Geneva, Switzerland: "Privileged Substructure Searching for Focused Set Design"

This year, the winning speaker was Mr. Nitin Rathore, a graduate student working with Prof. Juan J. de Pablo. He received a check for \$1000 sponsored by [Schrodinger, Inc.](#) In addition, all symposium speakers and the members of the Panel of Experts that made the selection were awarded a complimentary one-year subscription to the *Journal of Molecular Graphics and Modelling*. Elsevier Science sponsored the subscriptions, and Professor Andy Holder, editor of the journal, made the presentation.

The fourth annual symposium will be held at the New York National Meeting. Long abstracts are due to Curt Breneman by April 14, 2003. For more information and a history of the symposium, please visit the COMP Division website.

The Division's Own Journal



Editor Andrew
Holder reports on
JMGM

Things are going
very well at
JMGM! Since

January 2002, I have received 52 new manuscripts. (The UK editorial office has handled even more.) The *Journal* is very definitely alive and well. We are pleased that both the quality and quantity of papers submitted is increasing. Topics of papers range from graphics algorithms through protein folding to the application of quantum mechanical methods. There is something in *JMGM* for every member of the Division. Two special issues are on the way as well—the topics will be announced at the ACS meeting in September in New York. Elsevier has now implemented electronic submission of manuscripts. This has certainly made things easier, and has significantly streamlined the review and publication process. Take a look at the website:

<http://www.elsubmit.com/esubmit/jmg>.

It is an exciting time to serve as your editor. Please let me hear from you any suggestions that you might have and, of course, **send me papers!**

Andy Holder

Upcoming Meetings & Symposia

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

- ACS Award for Computers in Chemical & Pharmaceutical Research
- Biological Applications of Implicit Solvent Models
- Computational Nanotechnology
- High-Throughput Computational Processes in Drug Discovery

- Integrating Diverse Computational Approaches to Complex Problem Solving
- Machine Learning in Computational Chemistry
- Multiple Length & Time Scales in Molecular Modeling
- Protein Flexibility
- Recent Developments & Applications of Time-Dependent DFT & Related *Ab Initio* and Semiempirical Methods
- Teaching Medicinal Chemistry & Drug Discovery to Undergraduate Chemistry Majors

Great Lakes Regional Meeting Chicago May 31 - June 2, 2003

A symposium in honor of Dr. John A. Pople, organized by Larry Curtiss of Argonne Labs, will be held this spring.

For more information, contact:
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Symposia for Future National Meetings:

New York, NY: September 7-11, 2003

- Computational and *in vitro* ADME Data: What is it Worth and How to Use It?
- Challenges for the Chemical Sciences in the 21st Century: Information & Communication
- Computational Chemistry in Drug Discovery: Are High Information Content Calculations Better Than Low Information Content Calculations?
- Emerging Technologies in Computational Chemistry
- Frontiers in DNA Research: An Interdisciplinary Symposium
- Parallel & High-Performance Computing in Chemistry

- The Challenge of Simulating Fluid Properties for Industry
- Theory & Simulation of Protein Folding Kinetics

Anaheim, CA: March 28-April 1, 2004

- Beyond Michael Dewar's Legacy: Modern Semiempirical MO Theory
- Interplay Between Computer Modeling & Experiments on Complex Biological Systems
- Nucleic Acid Modeling
- Rational Drug Design
- *In Silico* High-Throughput Screening
- Structure Based Design for Protein Families

COMP Division Web Site News

Visit the *COMP* website for all the details!

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

The web site continues to grow and improve. Over the last few months we have added:

- A link for electronic submission of manuscripts to the *Journal of Molecular Graphics and Modelling*
- Application deadlines and award recipient announcements for all COMP sponsored awards

The most up-to-date information on COMP programs can be found on the website. And if you're looking for something and don't find it, let me know and I'll do my best to get it on-line.

For those of you interested in using XML to transmit chemical data, check out <http://www.xml-cml.org/> for the latest on chemical markup language (CML), which has recently been upgraded to conform to the W3C specification for Schemas.

Lisa M. Balbes, WebMaven

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