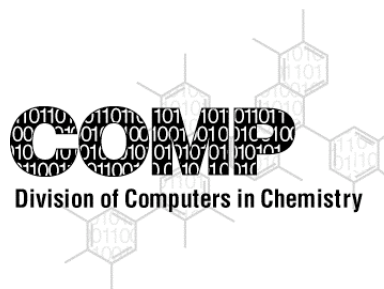


## Fall 2003 Highlights

- Ten students to receive Chemical Computing Group Excellence Awards in NYC
- Award winner to be selected during Emerging Technologies Symposium



# COMP Newsletter

## Statement from the Chair

*Peter Grootenhuis, the Chair of COMP, summarizes Division activities in 2003*

We look back on a very successful ACS national meeting in New Orleans. Despite the tensions and war in Iraq, the meeting and the many COMP symposia were well attended. This year Professor Ken Houk (UCLA) received the ACS Award for Computers in Chemical and Pharmaceutical Research for his many outstanding contributions to the field. The COMP poster session featured the presentation of Excellence Awards (10 this year!), generously sponsored by the Chemical Computing Group.

The upcoming meeting in New York will host exciting COMP symposia covering a diversity of topics such as ADME data modeling, structure-based design in signal transduction, protein folding kinetics, simulating fluid properties, and spin-forbidden and open-shell processes. As always, our Program Chair Ralph Wheeler and Vice Program Chair Wendy Cornell have done a tremendous job in the coordination and organization of these symposia.

Although the COMP Division is currently in good financial shape (carefully monitored by our Treasurer Curt Breneman), the Executive Committee has decided to raise the membership fees for 2004 to \$15 for regular ACS members. (The fees for student members will be \$10 per year). The increase is necessary for sponsoring the new initiative to produce an annual review of current areas of research within computational chemistry. David Spellmeyer, COMP's Director of Public Relations, is working hard to get everything organized. Although the details are being finalized, members can expect the first edition around December 2004. We hope that this initiative will further enhance the membership of the COMP Division. We will keep you posted on the progress we are making through these Newsletters and our website.

I look forward to seeing you in the Big Apple.

Peter Grootenhuis

### COMP Division Web Site News

*What's New on the Web?*

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

- Photos from the New Orleans meeting, courtesy of David Spellmeyer
- An announcement of the M.J.S. Dewar Symposium, written by Andy Holder
- Latest news of COMP awards and upcoming deadlines

### COMP Programming Notes

*Update from Ralph Wheeler, Program Chair*

Once again, symposium organizers have stepped forward to give the Division a strong program at the Fall ACS National Meeting. In addition to the usual slate of outstanding topical symposia, general contributions, and a poster session from 6pm–8pm Tuesday evening, I want to highlight three special symposia planned for this meeting. These are:

- (1) "Emerging Technologies in Computational Chemistry", an annual symposium supported by a \$1000 prize from Schrödinger, Inc. for the

Newsletter of the COMP division of the ACS  
Fall 2003

best contribution, organized by Curt Breneman

- (2) "Challenges for the Chemical Sciences in the 21st Century: Information and Communication", organized by Peter Gund—a summary of a National Research Council workshop to consider national research priorities in computational chemistry and chemical engineering
- (3) "The Challenge of Simulating Fluid Properties for Industry", a symposium organized by Ray Mountain to present the results of a competition in this field

At the Spring 2004 national meeting in Anaheim, CA, special symposia include the ACS Award for Computers in Chemical and Pharmaceutical Research and the Division's first endowed symposium in honor of an eminent chemist, M. J. S. Dewar. Topics will vary, but the first Dewar Symposium, organized by Tim Clark, will be entitled "Beyond Michael Dewar's legacy: modern semiempirical MO theory". Seed funding from Semichem, Inc. supports the Symposium, and additional funding will be gratefully accepted.

The COMP Division will also award Chemical Computing Group Excellence Awards to ten outstanding graduate students planning to present their work as part of the COMP program in Anaheim. Awards will pay travel expenses to the meeting and provide a one-year license for the CCG software package MOE. Applications—an extended abstract, vitae, personal statement, and a supporting letter from the student's advisor—are due to Curt Breneman by October 31, 2003. Please mark your calendars for the Anaheim meeting March 28–April 1, 2004, and note the OASYS abstract submission deadline (as of this writing) is November 15, 2003.

See you in New York City!

Ralph Wheeler

### Preview of the Emerging Computational Technologies Symposium

### Award will be presented at the New York ACS national meeting

You are invited to attend the fourth annual Symposium on Emerging Computational Technologies, Tuesday afternoon, September 9<sup>th</sup>. The objective of the symposium is to stimulate, reward, and publicize methodological advances in computational chemistry.

From the applications received, members of a Panel of Experts selected seven speakers. At the symposium, the talks will be evaluated by the Panel based on the impact the research will have on the future of computational chemistry and allied sciences. A prize of \$1000 generously sponsored by Schrödinger, Inc, will be presented to the selected speaker, and Elsevier Science will provide free one-year subscriptions to the *Journal of Molecular Graphics and Modelling* to symposium participants.

The Emerging Technology presentations and contenders are:

- "Mining molecular dynamics data for molecular properties", **Ralph A. Wheeler** (University of Oklahoma)
- "A super-linear minimization scheme for the nudged elastic band method", **Jih-Wei Chu** and Bernhardt Trout (Massachusetts Institute of Technology), and Bernard R. Brooks (National Institutes of Health)
- "Peptide to non-peptide: A real breakthrough in virtual screening", **Jeremy G. Vinter**, Timothy J. Cheeseright, and Mark D. Mackey (Crescent BioMolecular Discovery)
- "Implementation and development of the self-consistent charge density functional tight-binding method", **Maciej Gutowski** (Pacific Northwest National Laboratory)
- "Prediction and classification of protein binding sites", **Matthias Keil** (Tripos, Inc.), and Thomas Exner & Jürgen Brickman (Darmstadt University of Technology)

- "QSAR-based database mining: A success story of the discovery and experimental validation of novel anticonvulsant compounds", **Min Shen**, Cecile Beguin, Alexander Golbraikh, Harold Kohn, and Alexander Tropsha (University of North Carolina at Chapel Hill)
- "Stochastic proximity embedding—methods and applications", **Huafeng Xu** and Dimitris K. Agrafiotis (3-Dimensional Pharmaceuticals, Inc., now Johnson & Johnson)

### 226th National ACS Meeting New York, NY Sept. 7-11, 2003

#### COMP—Co-sponsored Symposia and Related Symposia of Interest

If you are attending the NYC meeting and the COMP program only whets your appetite for talks in the area of "Computers in Chemistry", you might consider the following symposia sponsored by other divisions...

**CHED:** Qualitative and Quantitative Assessment of Molecular Modeling in the Undergraduate Curriculum

**CINF:** Using Protein Structures and Signaling Pathway Information in Compound Design (with BIOT, COMP, MEDI)

**TOXI:** Computational Toxicology (with COMP)

**COLL:** Computer Simulations in Surface and Colloid Science

**FUEL:** Computer Modeling and Simulation in Fuel Chemistry and Catalysis

**FUEL:** Reaction Pathways and Structure-Property Relationships in Fuel Chemistry

**INOR:** Bioinorganic Modeling

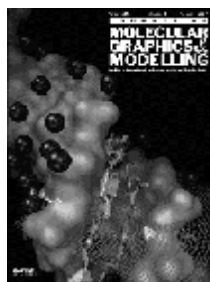
**INOR:** Computational Inorganic Chemistry

**MEDI:** Protein Families as Targets (with COMP)

**PHYS:** Making and Breaking Chemical Bonds in Gas and Condensed Phases: Theory and Applications

**PHYS:** Quantum Monte Carlo Methods

### *Journal of Molecular Graphics and Modelling*



*The COMP Division's Journal*

It has been a strong year for the Journal and we are increasing both in quality and quantity of articles submitted. I want to express appreciation for all of the members who have submitted papers and who serve on the Editorial Board and as referees—it really has become the “Division’s Own Journal”. The electronic submission system is up and running and we are please with how it has streamlined the publication process. Take a look at the website: <http://www.elsubmit.com/esubmit/jmg>.

Also, please note that Elsevier will be supporting its first sponsored symposium at the meeting in Anaheim, and this will result in a special issue of the Journal.

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

### Chemical Computing Group Excellence Award Recipients Announced



### Chemical Computing Group Excellence Awards support travel for 10 students

The ACS Division of Computers in Chemistry and the Chemical Computing Group are pleased to announce the latest recipients of the CCG Excellence Awards for the Fall 2003 meeting in New York. Congratulations to the Awardees!

- **Ghosh, Tuhin**, *Rensselaer Polytechnic University, Department of Chemical Engineering*: “Proteins under stress: molecular studies of pressure effects on proteins”
- **Mattioni, Brian**, *Pennsylvania State University*: “Classifying the mutagenicity of two diverse sets of organic compounds using Ames test data for *Salmonella typhimurium* TA100 and TA98”
- **Rathore, Nitin**, *University of Wisconsin, Madison*: “Density of states simulations of proteins in a continuum”
- **Shen, Ling-Ling**, *Rensselaer Polytechnic University Department of Chemistry*: “Modeling the mu-opioid receptor affinity of synthetic 8-aminocyclazocine analogues using TAE, PEST, and PAD descriptors and machine-learning methods”
- **Shen, Min**, *University of North Carolina, Chapel Hill*: “Discovery and experimental validation of novel functionalized amino acid anticonvulsant compounds: a success story of QSAR-based database mining”
- **Thompson, Jason**, *University of Minnesota*: “Predicting aqueous solubility: a fundamental approach”
- **Tschampel, Sarah**, *University of Georgia*: “Rational development of a lone pair inclusive force field”
- **Udier-Blagovic, Marina**, *Yale University*: “Validation of a model for the complex of HIV-1 reverse

transcriptase with non-nucleoside inhibitor TMC125”

- **Wang, Dong-qi**, *University of Hong Kong*: “A DFT investigation of the remarkable reactivity of the *gem*-dizinc carbenoid  $(IZn)_2CHI$  as a cyclopropanation reagent with ethylene compared to its mono zinc carbenoid  $IZnCHI_2$ ”
- **Wu, Yudong**, *Princeton University*: “Application of a coarse-grained dynamical method to explore the conformational space of small molecules”

The CCG Excellence Awards were established in 2000 to stimulate graduate student participation in COMP Division symposia and poster sessions at ACS National Meetings. Awardees are chosen on the basis of the quality and significance of the research to be presented and the strength of the supporting materials. These students receive a one-year software license of CCG’s MOE (Molecular Operating Environment) for their academic research groups, in addition to travel costs, and are recognized at the Division’s Tuesday evening poster session at each meeting.

Details regarding the application process for the Spring 2004 meeting in Anaheim are posted on the COMP Division web site.

### Upcoming ACS National Meetings

#### Current List of Symposia & Organizers

#### Anaheim, Spring 2004:

- 1) Beyond Michael Dewar’s Legacy: Modern Semiempirical MO Theory (Tim Clark, Erlangen University)
- 2) G-Protein Coupled Receptor Structure, Modeling, and Ligand Design (Irache Visiers, Millenium Pharmaceuticals; John Woolfrey, Cor Therapeutics)
- 3) Interplay Between Computer Modeling and Experiments on Complex Biological Systems (Ron Levy, Rutgers University)
- 4) Nucleic Acid Modeling (Neocles Leontis, Bowling Green State University)
- 5) QSAR (Bob Clark, Tripos, Inc.)

6) Rational Drug Design (Rami Reddy, Metabasis Therapeutics Inc.)

**Philadelphia, Fall 2004:**

1) Symposium in Honor of Henry F. Schaefer's 60<sup>th</sup> Birthday (Paul Von Rague Schleyer, University of Georgia; Ernest Davidson: University of Washington; Weston T. Borden, University of Washington)

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