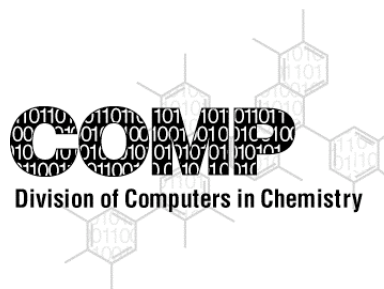


## Spring 2004 Highlights

- All Week in Anaheim: Inaugural Symposium in Honor of M. J. S. Dewar
- Graham Richards to be Honored Tuesday Afternoon with ACS Award for Computers in Chemical & Pharmaceutical Research
- COMP Poster Session & Social Hour Tuesday Evening—Division's CCG Excellence Awards will be Presented to 10 Students



# COMP Newsletter

## COMP Elections, Past and Future

### *Five New Officers Elected in 2003*

The last Division election is complete and was successful! We have elected a number of key individuals that will continue to make the COMP Division even better. Five new officers were elected this year. Andy Holder was elected as the 2004 Chair-Elect. Andy has strong COMP experience, having served as secretary for the COMP Division for three years and organized four symposia at national ACS meetings and two at regional ACS meetings. He also currently serves as the US editor for the *Journal of Molecular Graphics and Modelling*.

Since the COMP division continues to grow, we have elected one additional councilor for this year, beyond our previous allocation of three positions! Not only was Peter Jurs re-elected, but David Spellmeyer was also elected as COMP's fourth councilor. Both Peter and David have extensive ACS experience and will undoubtedly serve the division well. Peter has served as an elected councilor for COMP for more than twenty years (1979-present). He served as a member of the ACS Society Committee on Chemical Abstracts Service from 1982-1990 and since then has served on the Joint Board-Council Committee on

Publications, where he is currently Vice-Chair. David has served the COMP Division as Chair-Elect, Chair, and Past-Chair from 2000–2002. He has organized two symposia on computational aspects of combinatorial chemistry (1995 and 1999 ACS Anaheim meetings) and served on the advisory board for an ACS educational tele/video conference series. David organized and hosted one of these conferences (Combinatorial Chemistry and the Medicinal Chemist: Is it a Match?), and has presented in another. Currently, David is leading the effort on the COMP division's new publication, the Annual Reports in Computational Chemistry.

The new Alternate Councilors starting this year are Ralph Wheeler and Jeffry Madura. Ralph has served as Program Chair for the COMP Division for the past four years, where he has been responsible for making the COMP Division's programming first-rate and a model for other ACS divisions. During his tenure, the number of COMP presentations at national meetings has grown from 170 to a record 492, which is incredible! Jeffry has considerable experience with COMP and PHYS divisions, as well as the Theoretical sub-division of PHYS. At the national level, Jeffry was a symposium organizer in the COMP Division for "Computational Chemistry in the Classroom" (1998 Boston meeting). He was also the 1996 Vice-Chair

for the Computational Chemistry Gordon Research Conference and the 1998 Chair.

As the COMP Secretary, I believe that we have elected outstanding individuals that will make significant contributions to the Division. Believe it or not – it's that time of year again, so please be ready to vote in the 2004 elections. Your vote matters – we typically have a 13% turn out. *Please vote as soon as you receive the ballot, which should arrive in the mail in May!* And if you'd like to get more involved with COMP in the future, please contact an officer—there are plenty of opportunities!

Jeff Evanseck

### **Deadlines for Philadelphia ACS National Meeting**

CCG Excellence Award Applications

*April 9, 2004*

OASYS Abstract Submissions for COMP Division Program

*April 16, 2004*

## Letter from the Program Chair

### *Ralph Wheeler concludes his term as Program Chair*

The Spring ACS National Meeting will be my last meeting as COMP Division Program Chair. While the job has been a lot of work, it has also been fun to meet new people, learn new science, and see such a growth in the number of symposia, the amount of funding for symposia, and the continued corporate sponsorship and endowment of regularly scheduled COMP Division events.

I especially want to thank the many symposium organizers who have done such a fantastic job taking care of everything from dimming the room lights during talks to raising funding for their symposia. It truly is the symposium organizers who make COMP programming great! Once again, our symposium organizers and corporate sponsors have come through to provide a strong COMP Division program in Anaheim. In addition to the usual slate of outstanding topical symposia, general contributions, and a poster session from 6-8 pm Tuesday evening, I want to highlight three special symposia planned for the Anaheim meeting. These are:

- (1) the "ACS Award for Computers in Chemical and Pharmaceutical Research" symposium, honoring Graham Richards, organized by Bill Jorgensen, and supported by a generous contribution from Accelrys, Inc.
- (2) the COMP Division's first endowed symposium in honor of an eminent chemist, M.J.S. Dewar. Symposium topics will vary, but the first Dewar Symposium, organized by Tim Clark, is entitled "Beyond Michael Dewar's legacy: modern semiempirical MO theory". The Dewar Symposium is supported by seed funding from Semichem Inc. Individuals or corporations wishing to provide additional support should contact the COMP Division's Treasurer, Curt Breneman.

- (3) a symposium organized by Douglas Tobias, entitled "Computational Approaches to Problems in Environmental Chemistry". This Elsevier-sponsored symposium is scheduled to become an annual event with rotating topics, so look for this symposium next year.

In addition to the corporate sponsors of these symposia, I also wish to single out the Chemical Computing Group for sponsoring the CCG Excellence Awards to graduate students, Hewlett-Packard for funding refreshments during our poster sessions, and the sponsorship by Schrodinger Inc. of our annual Emerging Technologies symposium. My heartfelt thanks go out to all of you for expressing your faith in the quality of COMP programming and your commitment to its continued success.

Although this is my last meeting as COMP Division Program Chair, I am passing responsibility for divisional programming into the capable hands of the new Program Chair, Wendy Cornell of Novartis Pharmaceuticals. Over the past four years as Vice Chair, Wendy has helped me through one major crisis and many smaller ones, so I know that the programming will continue to improve. Thanks, Wendy, and best wishes!

Thanks to you all! It's been a privilege and a pleasure serving you!

Ralph A. Wheeler

### ACS Award for Computers in Chemical & Pharmaceutical Research

Professor W. Graham Richards, Chairman of the Chemistry Department at Oxford University, will receive the ACS Award for Computers in Chemical and Pharmaceutical Research Tuesday afternoon, March 30<sup>th</sup>. This award, sponsored by Accelrys Inc., recognizes outstanding contributions to the advancement of the use of computers in the chemical and biological sciences.

Richards received his undergraduate and graduate degrees at Oxford, where he has since continued his scientific career. His research group has developed and

applied computational methods for drug design, molecular similarity analysis and protein structure prediction, and performed simulations of enzyme reaction mechanisms, DNA recognition, and lipid bilayers. Recent efforts have included the "Screensaver Lifesaver" project, exploiting available personal computer cycles on millions of volunteered computers to screen molecules for anticancer activity. More details on this project may be found at:

<http://www.chem.ox.ac.uk/curecancer.html>

The award address is entitled "From Diatomics to Drugs to Distributions" and will conclude the symposium, which also features presentations by J. Andrew McCammon, Richard Lavery, William Jorgensen, and Meir Glick.

### Emerging Technologies in Computational Chemistry Symposium

#### *Fifth Annual Symposium to be Held in Philadelphia - Abstracts due April 16th*

The objective of the Symposium on Emerging Technologies in Computational Chemistry at the Fall annual ACS meeting is to stimulate, reward, and publicize methodological advances in computational chemistry. The talks will be evaluated by a Panel of Experts based on the impact the research will have on the future of computational chemistry and allied sciences. The symposium will be ideal for presenting your latest and best research on new techniques and software development, and Schrodinger, Inc., will again sponsor a \$1000 prize for the best talk at the symposium.

All are invited to participate. To do so, it is necessary to submit a regular short ACS abstract via <http://oasys.acs.org/> by April 16, 2004. It is also necessary to email a more detailed (~1000-word) abstract to me by the same date. 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 Emerging Technologies Symposium that cannot be accepted will be rescheduled in one of the other COMP sessions at the meeting.

Curt M. Breneman

## Chemical Computing Group Excellence Award Winners Announced



Ten Students to be Recognized with CCG Excellence Awards Tuesday Evening

The COMP Division will grant Chemical Computing Group Excellence Awards to ten outstanding graduate students presenting their work as part of the COMP program in Anaheim. Awards subsidize travel expenses to the meeting and provide a one-year license for the CCG Molecular Operating Environment (MOE) software (<http://www.chemcomp.com/>).

The awardees, in alphabetical order, are:

- Andreas Bender: "Similarity Searching using Atom Environments, Information Gain-based Feature Selection and the Naïve Bayesian Classifier", *University of Cambridge*
- Xiaolin Cheng: "Molecular Dynamics Simulations of 8-oxoguanine: A Mismatch DNA", *State University of New York, Stony Brook*
- Wei (David) Deng: "Predicting Protein-Ligand Binding Affinities using Transferable Atom Equivalent (TAE) Techniques and Machine-Learning Methods", *Rensselaer Polytechnic Institute*
- Asif Ladiwala: "Prediction of Protein Affinity in Hydrophobic Interaction Chromatography using Quantitative Structure-Retention Relationship (QSRR) Models", *Rensselaer Polytechnic Institute*
- Anne E. Loccisano: "Development of New CHARMM Force Field Parameters for Novel DNA Bending Agents", *Duquesne University*

- Asim Okur: "Multiple Pathways in Beta-Hairpin Folding and Unfolding Simulations", *State University of New York, Stony Brook*
- Alexander Perryman: "HIV-1 Protease Molecular Dynamics of a Wild-Type and of the V82F/I84V Mutant: Possible Contributions to Drug Resistance and a Potential New Target Site for Drugs", *University of California, San Diego*
- Sarah A. Mueller Stein: "The Influence of Steric Congestion on the Dynamics and Geometry of DNA", *Duquesne University*
- Jessica Swanson: "Revisiting Free Energy Calculations: One Step Closer to Rigorous Scoring Functions and One Step Beyond MM/PBSA", *University of California, San Diego*
- Ivan Tubert-Brohman, "Improved Semiempirical Methods: Parameterization of PDDG/PM3 for Sulfur", *Yale University*

Applications for Awards to attend the meeting in Philadelphia in August consist of an extended abstract, vitae, personal statement, and a supporting letter from the student's advisor and are **due to Curt Breneman before April 9, 2004**. Please see the COMP website for more details.

### COMP Division Web Site News

*New Format for the COMP Website*

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

The COMP division web site has been completely re-designed. The new version can be seen at the address above and features current events on the home page, a navigation menu on each page, and more. Check it out for yourself and see all the latest COMP news! Please continue to send your suggestions and additions to [lisa@balbes.com](mailto:lisa@balbes.com) - we want to know what you want.

Lisa M. Balbes, WebMaven

### Online Conference

"Teaching Computing in Chemistry Courses"

The ACS Division of Chemical Education's Committee on Computers in Chemical Education (CCCE) is soliciting papers for an online conference that will be held September through October 2004. This conference will highlight what and how computing is taught in chemistry courses and consider questions like:

- What do chemistry students need to learn about computers and computing?
- When and how should this information be taught?
- What should be taught in required courses?
- What should be taught in elective courses?

Papers are suggested that describe either computer courses that are taught in Chemistry, or computer subject matter taught in traditional chemistry courses. Papers might include one or more of the following topics: website development, web resources and searching the web, spreadsheets, graphics, word processing, PowerPoint and/or other presentation tools, programming, numerical and statistical methods, computation and molecular modeling, and information about hardware and software.

#### Deadlines:

Titles and abstracts: July 1, 2004  
Papers submitted: August 1, 2004

For additional information consult the CONFICHEM website or contact one of the Conference organizers:  
<http://www.ched-cce.org/confchem/notes.html>

Carl H. Snyder, University of Miami  
Email: [csnyder@miami.edu](mailto:csnyder@miami.edu)  
Phone: (305) 284-2174

Donald Rosenthal, Clarkson University  
Email: [rosen@clarkson.edu](mailto:rosen@clarkson.edu)  
Phone: (315) 265-9242

## Symposia: National ACS Meetings

### 227th National ACS Meeting Anaheim, CA: March 28-April 1, 2004

#### Sponsored by COMP...

- Beyond Michael Dewar's Legacy: Modern Semiempirical MO Theory
- Interplay Between Computer Modeling & Experiments on Complex Biological Systems
- Getting it Right: Variable Selection and Model Validation in (Q)SAR
- G-Protein Coupled Receptor Structure, Modeling, and Ligand Design
- Nucleic Acid Modeling
- Rational Drug Design
- Computational Approaches to Problems in Environmental Chemistry
- Computers in Chemistry: General Contributions

#### ... and in Other Divisions

- Computational Chemistry of Carbohydrates (CARB)
- What's the Next Big Step for Using Computers to Teach Chemistry (CHED)
- The Bigger Picture: Linking Bioinformatics to Cheminformatics (CINF)
- Research Collaboratories, Virtual Laboratories, and Grid Computing (CINF)
- Informatics Challenges in Nanotechnology (CINF)
- Advances in Pharmacophores and 3D Searching (CINF)
- Molecular Modeling and Reaction Chemistry (FUEL)
- Bioinorganic Modeling (INOR)
- Computational and Experimental Chemistry (INOR)
- Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry & High-energy Species (ORGN)
- Intermolecular Interactions & Reactions Involving Ions and Open-shell Systems (PHYS)

## COMP Wants You!

The Executive Committee is looking for people interested in helping COMP organize symposia, to work with the national ACS and its council, and to develop strategic plans for our members beyond our excellent programming. If you'd like to learn more, contact our Chair, Michelle Francl. Committee meetings are held the Saturday afternoon of each National ACS Meeting and visitors are welcome!

- Mixed Quantum, Classical & Semi-classical Dynamics (PHYS)
- Protein Structure Prediction & Folding: Where Physical Chemistry Meets Genomics (PHYS)
- Industrial Applications of Theoretical Chemistry (PHYS)

#### Philadelphia, PA: Aug. 22-26, 2004

- Emerging Technologies in Computational Chemistry
- Computational Chemistry in the Discovery and Development of New Anti-Infective Agents
- Docking and Scoring: Novel Methods, Evaluations, and Improvements
- Symposium in Honor of Henry F. Schaefer's 60th Birthday
- 3-D Visualization Technology for Teaching Chemistry
- High Performance Computing for Computational Chemistry
- Molecular Modeling in Environmental Chemistry (ENVR, GEOC)

#### San Diego, CA: March 13-17, 2005

- ACS Award for Computers in Chemical and Pharmaceutical Research
- Modeling Protein-Ligand Interactions

#### Washington, DC: Aug. 28-Sept. 1, 2005

- Emerging Technologies in Computational Chemistry
- Computational Study of Liquids and Liquid Interfaces

## Regional ACS Meetings

The Office of Regional Meetings (ORM) has released its schedule for 2004. Please visit the ORM website to link with the individual meetings for more details at [www.acs.org/meetings/regional](http://www.acs.org/meetings/regional).

Most regional meetings have programming related to computational chemistry, and COMP Division members are encouraged to participate. For example, CRM 2004 will feature a general computational chemistry session and symposia on "Computational Solutions to Alzheimer's Disease" (Don Boyd, Indiana University-Purdue University Indianapolis, chair) and "Where Do We Go Next with Docking and Scoring Methodologies?" (Michal Vieth, Lilly Research Laboratories, organizer).

Abstracts and registration are now open for the June meetings, but the deadlines for both are in the next two weeks, so make your plans today!

### Summer

#### Central (CRM 2004)

June 2-5, Indianapolis, IN

#### Northwest/Rocky Mountain (NORM/RMRM 2004)

June 6-9, Logan, UT

### Fall

#### Southwest (SWRM 2004)

Sept. 29-Oct. 2, Fort Worth, TX

#### Great Lakes (GLRM 2004)

Oct. 17-20, Peoria, IL

#### Midwest (MWRM 2004)

Oct. 19-22, Manhattan, KS

#### Western (WERM 2004)

Oct. 27-30, Sacramento, CA

#### Northeast (NERM 2004)

Oct. 31-Nov. 3, Rochester, NY

#### Southeast (SERMACS 2004)

Nov. 10-13, Raleigh/Durham, NC

## COMP Division Contact Information

**Chair:** Michelle Francl  
Bryn Mawr College, Dept. of Chemistry  
Phone: (610) 526-5108  
Email: [mfrancl@brynmawr.edu](mailto:mfrancl@brynmawr.edu)

**Past Chair:** Peter D. J. Grootenhuis  
Vertex Pharmaceuticals  
Phone: (858) 404-6676  
Email: [Peter\\_Grootenhuis@sd.vrtx.com](mailto:Peter_Grootenhuis@sd.vrtx.com)

**Chair-Elect:** Andrew Holder  
University of Missouri-Kansas City, Dept.  
of Chemistry  
Phone: (816) 235-2293  
Email: [holdera@umkc.edu](mailto:holdera@umkc.edu)

**Treasurer:** Curt Breneman  
Rensselaer Polytechnic University,  
Dept. of Chemistry  
Phone: (518) 276-2678  
Email: [brenec@rpi.edu](mailto:brenec@rpi.edu)

**Secretary:** Jeffrey D. Evanseck  
Duquesne University, Dept. of Chemistry  
and Biochemistry  
Phone: (412) 396-6337  
Email: [evanseck@duq.edu](mailto:evanseck@duq.edu)

**Program Chair:** Wendy Cornell  
Novartis Pharmaceuticals  
Phone: (908) 277-7524  
Email:  
[wendy.cornell@pharma.novartis.com](mailto:wendy.cornell@pharma.novartis.com)

**Program Chair:** Ralph Wheeler  
University of Oklahoma, Dept. of  
Chemistry & Biochemistry  
Phone: (405) 325-3502  
Email: [rawheeler@chemdept.chem.ou.edu](mailto:rawheeler@chemdept.chem.ou.edu)

**JMGM Liaison:** Andrew Holder  
University of Missouri-Kansas City, Dept.  
of Chemistry  
Phone: (816) 235-2293  
Email: [holdera@umkc.edu](mailto:holdera@umkc.edu)  
**WebMaven:** Lisa M. Balbes  
Balbes Consultants  
Phone: (314) 966-5298  
Email: [lisa@balbes.com](mailto:lisa@balbes.com)

**Newsletter:**  
Michelle L. Lamb  
AstraZeneca R&D Boston  
Phone: (781) 839-4000  
Email: [michelle.lamb@astrazeneca.com](mailto:michelle.lamb@astrazeneca.com)

### Public Relations & Editor, Annual Reports in Computational Chemistry:

David Spellmeyer  
IBM Almaden Services Research  
Phone: (408) 927-1933  
Email: [dspell@us.ibm.com](mailto:dspell@us.ibm.com)

### Councilors & Alternate Councilors:

Peter C. Jurs  
Penn State University, Chemistry Dept.  
Phone: (814) 865-3739  
Email: [pcj@psu.edu](mailto:pcj@psu.edu)

Michelle Francl  
Bryn Mawr College, Dept. of Chemistry  
Phone: (610) 526-5108  
Email: [mfrancl@brynmawr.edu](mailto:mfrancl@brynmawr.edu)

Jennifer Miller  
Consultant  
Phone: (650) 326-7546  
Email: [jmiller@idiom.com](mailto:jmiller@idiom.com)

David Spellmeyer  
IBM Almaden Services Research  
Phone: (408) 927-1933  
Email: [dspell@us.ibm.com](mailto:dspell@us.ibm.com)

Peter Gund  
Accelrys, Inc.  
Phone: (609) 452-3610  
Email: [pgund@accelrys.com](mailto:pgund@accelrys.com)

Hanneke Jansen  
Chiron Corporation  
Phone: (510) 923-4062  
Email: [hanneke\\_jansen@chiron.com](mailto:hanneke_jansen@chiron.com)

Jeffry Madura  
Duquesne University, Department of  
Chemistry and Biochemistry  
Phone: (412) 396-4129  
Email: [madura@duq.edu](mailto:madura@duq.edu)

Ralph Wheeler  
University of Oklahoma, Dept. of  
Chemistry & Biochemistry  
Phone: (405) 325-3502  
Email: [rawheeler@chemdept.chem.ou.edu](mailto:rawheeler@chemdept.chem.ou.edu)