



Press Release

April 9, 2002

CCG Excellence Award Winners Announced at the Spring 2002 National ACS Meeting in Orlando

MONTREAL and ORLANDO, April 9, 2002 -- The American Chemical Society (ACS) Division of Computers in Chemistry (COMP) and Chemical Computing Group (CCG), are pleased to announce the winners of the CCG Excellence Awards for the Spring ACS National Meeting, held in Orlando, FL from April 7-11, 2002. The awards were first created two years ago by CCG in conjunction with the COMP division. They were created to stimulate graduate student participation in COMP division activities (symposia & poster sessions) at ACS National Meetings. Winners receive a one-year software license of CCG's MOE (Molecular Operating Environment) for their academic research groups, in addition to reimbursement for travel costs associated with attending an ACS National Meeting to present their research.

"We are very pleased with CCG's continued support of the student awards. The program continues to allow deserving students to present their work at the National ACS meeting and to interact with prominent scientists in the area of computational chemistry," stated Dr. Bill Jorgenson, Chair of the COMP division.

In alphabetical order, the winners are:

- Thomas Dick, Duquesne University in Pittsburgh, PA for his poster: *Computational Modeling of Brine to aid CO2 Sequestration Research*. Advisor: Jeffry Madura.
- Benoit Leblanc, Institut Francais du Petrole in Reueil-Malmaison, France for his poster: *Mixing Monte Carlo moves more efficiently with an evolutionary algorithm*. Advisors: Herve Toulhoat, Bertrand Braunsweig & Evelyne Lutton.
- Viera Lukacova, North Dakota State University for her poster: *Implementation of Multiple Binding Modes in CoMFA*. Advisor: Stefan Balaz.
- Sabine Schefzick, Indiana University-Purdue University-Indianapolis (IUPUI) for her poster: *Theoretical Ligand Distortions in Chiral Catalysts: Can molecular deformations enhance a catalyst's chirality content?* Advisor: Kenny Lipkowitz.
- Xuelin Wang, University of North Texas for his poster: *Error Analysis in Density Functional Theory: Atomization Energies*. Advisor: Angela K. Wilson.

Awardees are chosen on the basis of the quality and significance of the research to be presented and the strength of the supporting materials. Please join us in

congratulating the winners on Tuesday April 9th, 2002, at the COMP General Poster Session held in Hall C at the Orange County Convention Center between 7:00 p.m. and 10:00 p.m.

Applications for the next round of CCG Excellence Awards (Boston - August 2002) are currently being accepted. The deadline for submission is Friday April, 26, 2002. All graduate students are encouraged to submit applications for the Awards. Students from the same research group are encouraged to apply. Students from research groups that have won awards at previous ACS meetings are also encouraged to submit applications. For more information please visit: <http://www.acs.org/meetings/boston2002>.

ABOUT CCG:

Chemical Computing Group (<http://www.chemcomp.com>) develops and markets MOE, the Molecular Operating Environment, a leading application for chemical researchers in the pharmaceutical and biotechnology fields. Its built-in applications cover the spectrum of drug discovery including: Protein/Homology modeling, High Throughput Screening, Combinatorial Library Design, Modeling/Simulations and Methods Development. MOEs unique architecture and platform independence allows it to be used corporate-wide by a variety of researchers - from methods developers to computational experts to medicinal chemists. Its customers include a worldwide roster of leading pharmaceutical and biotechnology companies.