



2006 Press Release

Chemical Computing Group Announces Excellence Award Winners at the 2006 ACS in Atlanta, GA.

MONTREAL, January 11, 2006 - Chemical Computing Group (CCG) and the American Chemical Society's (ACS) Division of Computers in Chemistry (COMP) congratulate winners of the CCG Excellence Awards at the 231st ACS National Meeting in Atlanta, Georgia.

The esteemed CCG Excellence Award honors graduate students in the field of computational chemistry. Winners are selected according to the excellence and relevance of their research, as well as the quality of the supporting materials. CCG is proud to award each winner a check to assist with travel and accommodation at the Fall 2006 ACS in Atlanta Georgia, recognition of their award-winning work at the Awards Presentation during the COMP Division Poster Session on Tuesday March 28, 2006, and a one-year software license for the latest version of MOE – the Molecular Operating Environment.

For more information on how to submit for the 2006 ACS Award in San Francisco, please contact Andrew Good at Andrew.Good@bms.com

2006 ACS Atlanta, GA Winners:

Xihua Chen, Yingkai Zhang, and John ZH. Zhang

“MFCC-DM with pairwise interaction correction quantum chemical study of proptein”, *New York University*

Xuhui Huang, Pu Li, Ruhong Zhou, and BJ. Berne

“Hydrophobic-Aided Replica Exchange: an efficient algorithm for sampling biological systems in explicit solvent”, *Columbia University*

Casey P. Kelly, Christopher J. Cramer, and Donald G. Truhlar

“Calculation of acid dissociation constants by the SM6 quantum mechanical implicit solvation model” *University of Minnesota*

Valerie McCarthy and Kenneth D Jordan

“Stability of Clathrates vs Cavity Occupancy”, *University of Pittsburgh*

Devina Pillay and Gyeong S Hwang

“Role of Oxygen Vacancies on Growth of 1B (Au, and Cu) Particles on TiO₂(110)”,
University of Texas, Austin