



Collaborative Graduate Specialization in
**Computational
Science and Engineering**

WEEKLY COLLOQUIUM

Tuesday, 28 November 2006

2:30-3:30 in Goodes 303

Speaker: NATALIE CANN
Associate Professor, Department of Chemistry
Queen's University

Title: Simulating chiral fluids and interfaces

Abstract: The talk will begin with a brief introduction to the importance of chiral (mirror-image) molecules. I will then focus on two projects where high performance computing has been essential: the structure, solvation, and selectivity of chiral stationary phases; and the development of polarizable, flexible molecular models. The former is directed at understanding the factors which lead to discrimination of mirror-image molecules, while the latter targets the impact of chiral molecules on their molecular environment. I will discuss some of the computational challenges we have faced in our simulations and the strategies we have used to deal with them.

About the speaker:

Natalie Cann received her Ph.D. in theoretical chemistry under the supervision of Russ Boyd (Dalhousie) and Ajit Thakkar (UNB). In 1993, she took up a postdoctoral position at the University of British Columbia with Gren Patey and Chris Brion. She joined the department of chemistry at Queen's in 1997, as a Queen's National Scholar.

Dr. Cann is a member of the HPCVL technical advisory committee, a co-applicant on an NSERC MFA grant supporting HPCVL, and a member of the selection committee for the Sun Microsystems of Canada Scholarship in Computational Sciences and Engineering.