

## Technical Workshop Series of the CENTRE FOR RESEARCH IN MOLECULAR MODELING

May 16, 2002 - Concordia University

### Path Integral Simulation Methods in Chemical Physics

Thursday, May 16, 2002. 10:00-16:00. H-1070

Guest Lecturer: Prof. Pierre-Nicholas Roy, Department of Chemistry, University of Alberta

1. Introduction to the path integral formulation of quantum mechanics
2. Real time propagation
  - a) The sign problem
  - b) Semi-classical approximations
  - c) Numerical example: the autocorrelation function and the power spectrum
3. Imaginary time propagation and statistical mechanics
  - a) Ensemble averages
  - b) Path Integral Monte Carlo techniques
  - c) Numerical example: The radial distribution function

Please register for the workshop by e-mailing us at [workshop@cermm.concordia.ca](mailto:workshop@cermm.concordia.ca)  
by Thursday, May 9, 2002.

Lunch will be provided.