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CERMM
Centre for Research in Molecular Modeling
Centre de Recherche en Modélisation Moléculaire

Joint Seminar Series of the
CENTRE FOR RESEARCH IN MOLECULAR MODELING, MERCK FROSST and the DEPARTMENT OF CHEMISTRY AND BIOCHEMISTRY

November 16th, 2007, 2:30 pm - Concordia University SP-S110

Quantum Molecular Dynamics of Large Molecular Systems

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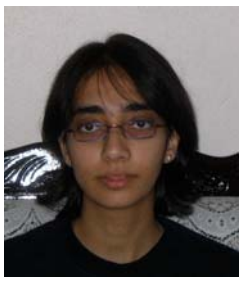
Classical molecular dynamics is a popular tool for probing the dynamical behaviour of atoms and molecules, particularly in systems of high dimensionality and complexity, through the integration of Newton's equations of motion. While it has seen widely successful applications in several disciplines, the technique is of limited use when investigating systems or phenomena of a quantum mechanical nature. For such problems, an accurate description of the dynamics is provided by quantum mechanics.

This seminar will introduce the broad field of molecular dynamics, both at the classical and quantum levels of theory. Specifically, the advantages and limitations associated with some of the popular methods will be discussed. One of the limitations is the prohibitively growing cost of exact quantum mechanical approaches, in general, with system size. As a result, alternative approximate techniques are needed for studying the dynamics of complex molecules. The seminar will focus on a particular method, based on semiclassical theory, which bears great promise for applications to large systems: the semiclassical initial value representation.

In an effort to further extend the applicability of semiclassical initial value representation to large complex systems practical and general approaches involving the introduction of geometrical constraints have been developed. Constraints lower the computational cost of calculations and hence enable the treatment of large molecules. Another key feature is generality, which is achieved via the use of the Cartesian coordinate system. The methods have been tested on atomic and molecular clusters. The ability of the techniques to accurately capture the desired quantum effect will be demonstrated through the calculation of zero-point energy.



Bilkiss Issack obtained a B. Sc. with Honours in Chemistry in 2000 from the University of Mauritius and a Ph. D. in Chemistry in 2007 from the University of Alberta, working on the development of semiclassical approaches for the dynamics of large complex molecular systems under the supervision of Prof. Pierre-Nicholas Roy. She is now a post-doctoral fellow in CERMM working with Gilles Peslherbe.