Concordia UNIVERSITY

MERCK FROSST
Merck Frosst Canada Inc., Kirkland, Québec, Canada

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

October 13, 2006, 2:30 pm - Concordia University SP-S110

Quantum Effects in Liquid Water

Dr. Lisandro Hernández de la Peña
Centre for Research in Molecular Modeling
Department of Chemistry & Biochemistry
Concordia University

This seminar will discuss how classical statistical mechanics fails to explain experimental differences between liquid H2O and D2O. A comprehensive introduction to quantum statistical mechanics in the path integral representation will be given, and the use of the “centroid molecular dynamics” (CMD) method to compute static and dynamical properties of a quantum system will be described. An extension of the original CMD method, that allows the direct quantization of the rotational motion in a molecular system, will be also presented.

The application of this (extended) version of the CMD method in the simulation of liquid water at ambient conditions will demonstrate that quantum effects are large. It will be shown that “quantum mechanical tunneling” occurs in water and the relationship between this and the mechanism of molecular diffusion will be established. Finally, it will be addressed how quantum effects change with temperature.

Lisandro Hernández de la Peña received his B.Sc. and M.Sc. degrees in Radiochemistry from the Institute for Nuclear Sciences and Technology (Havana, Cuba) in 1995 and 1997, respectively. After spending two years teaching undergraduate physical chemistry in Havana, he enrolled in the Chemistry Ph.D. program at Dalhousie University in the group of Prof. Peter Kusalik in 1999. He completed his Ph.D. in 2004 and joined the Chemical Physics Theory Group at the University of Toronto, working as a post-doctoral Fellow in the group of Prof. Jeremy Schofield. In the year 2006, Lisandro moved to Concordia University, where he currently is a post-doctoral Fellow in the Centre for Research in Molecular Modeling in the group of Prof. Gilles Peslherbe.