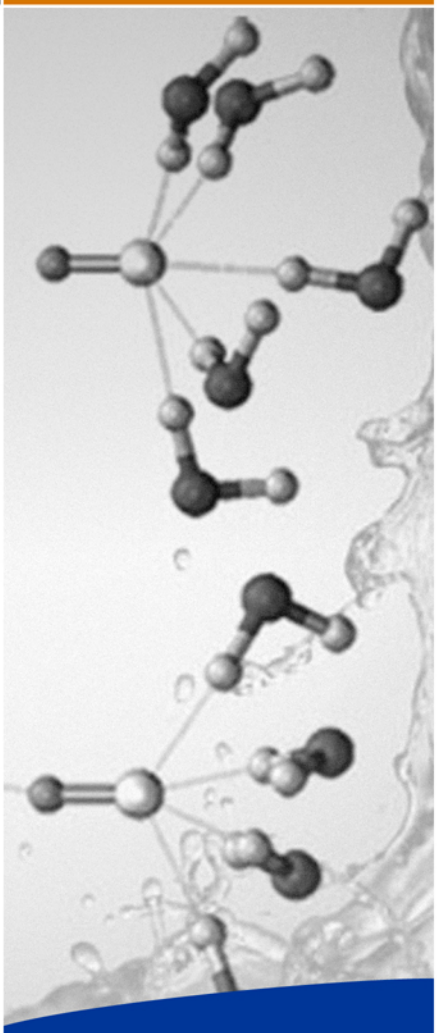
Competing Quantum Effects in Liquid Water

Pacific Northwest NATIONAL LABORATORY

Proudly Operated by Battelle Since 1965

Frontiers in Chemical Physics and Analysis Seminar Series



Presented by…

Professor David Manolopoulos

Physical and Theoretical Chemistry Laboratory
The University of Oxford

Abstract

I will begin this talk with a brief review of the ring polymer molecular dynamics (RPMD) method for condensed phase quantum dynamics. I will then use this method to investigate the properties of a flexible water model that has been parameterized to agree with a wide variety of experimental measurements in quantum mechanical (path integral) simulations. I shall show in particular that there is a competition between two opposing quantum mechanical effects in the dynamics of the room temperature liquid. The zero point motion in the intramolecular OH stretch increases the average OH bond length and the average dipole moment of the water molecules, leading to stronger intermolecular interactions and a more viscous liquid. However, this is offset by the zero point motion in the intermolecular modes, which disrupts the hydrogen bonding network and makes the liquid more labile again. The net result is that there is only a very small overall quantum mechanical effect in the self-diffusion and orientational relaxation of the liquid. If time permits at the end of the talk, I shall go on to discuss some related studies by other groups that support this picture.

More info?

See http://www.pnl.gov/cmsd/seminars/

Date: March 20th

Location: EMSL Auditorium

Time: 9:00 am