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Water on a Knife-Edge: The Subtle Balance of Forces in Clusters, Ice and Liquid

Frontiers in Chemical Physics and Analysis
Seminar Series

Presented by…

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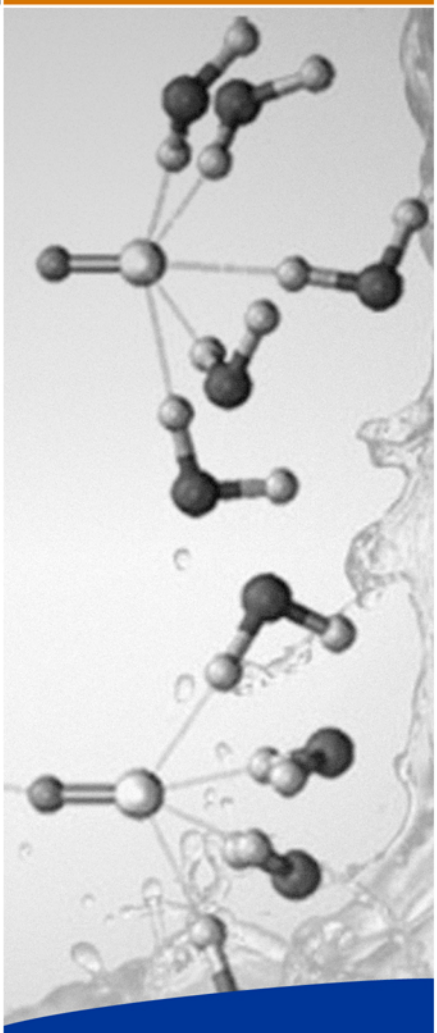
Water has probably been studied more comprehensively than any other substance, but its molecular-scale energetics remains surprisingly elusive. Parameterized interaction models, including some developed at PNNL, can be remarkably successful. But widely used electronic-structure methods based on conventional density-functional theory (DFT) struggle to reproduce the properties of water clusters, ice structures and the bulk liquid, for reasons that are still controversial. I will summarize some new approaches that we are pursuing at UCL in collaboration with colleagues at Cambridge and Bristol, focusing particularly on our recent work with quantum Monte Carlo (QMC) [1] and Gaussian Approximation Potentials (GAP) [2]. I will show that QMC is much more accurate than DFT for the energetics of clusters [3] and ice structures [4], and that it can also supply useful benchmarks for statistical samples of configurations of the bulk liquid. We are using QMC and correlated quantum chemistry techniques to analyze the sources of error in DFT approximations and to quantify the accuracy of GAP corrections to DFT. It is becoming clear from this work that conventional DFTs have a hard time describing water systems because they misrepresent the subtle balance between 2-body (dispersion) and beyond-2-body (polarization) parts of the energy.

More info?

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



Date: APR 27, 2012

Location: EMSL Auditorium

Time: 9:30 am