Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Discovery of Water Structural Transitions near Interfaces of Polarizable Solutes[1] MOHAMMADHASAN DINPAJOOH, DMITRY MATYUSHOV, Arizona State Univ — The standard harmonic approximation describing polarization around the solute is expected to break down with increasing solute polarizability. The focus of this study is to investigate the structure of water around dipolar-polarizable solutes by Monte Carlo (MC) simulations in the non-harmonic regime. We observe a structural transition in the water hydration shell and its condensation, which are driven by increasing the solute polarizability. There is also a crossover in the orientational structure near the point of breakdown of the harmonic approximation. At lower polarizabilities, waters in the hydration shell point their hydrogens toward the solute. The dipoles flip their orientations at the transition to the non-harmonic regime. Both the hydration shell compressibility and the electric field susceptibility display maxima in the transition region. Using the water electric field at the center of the polarizable solute as the order parameter, a Landau-type model is formulated. Its predictions are in reasonable agreement with MC simulations performed for hard sphere and Lennard Jones polarizable solutes in a TIP3P water model. The observed structural transition suggests a general crossover phenomenon driven by the stabilization energy required to polarize the solute.

[1]This research was supported by the National Science Foundation (CHE-1213288). CPU time was provided by the National Science Foundation through XSEDE resources (TG-MCB080116N).

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Date submitted: 16 Oct 2014 Electronic form version 1.4