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The CSI Chemistry Department Presents

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Understanding Water and Its Interactions with Biomolecules

Date: 4/11/2024 **Time: 2:30 PM** **Room: 6S-232**

In general, pure substances exists in one liquid state and, if crystallization is avoided, a single glass state is formed upon fast cooling. The properties of the glass that forms depend on both the cooling and compression/decompression rates. Experiments suggest that water is surprisingly different, having two different liquid states in the supercooled region, low density liquid (LDL) and high-density liquid (HDL), and two different glassy states, low density amorphous (LDA) and high density amorphous (HDA). These finding have far reaching effects for the potential application in cryogenic technology. In this talk I we will discuss the water liquid-liquid phase transition (LLPT) scenario in which LDL and HDL are separated by a first order phase transition line that ends in a liquid-liquid critical point (LLCP) and the relationship of this line to LDA and HDA. I will also discuss the “first order-like phase transition” between LDA and HDA. Computational studies will be presented that 1) show the existence of the LLCP, 2) how nuclear quantum effects (NQE) influence its location, and 3) how response thermodynamic functions vary with NQE in the supercritical region. Two models will be presented: 1) a simple coarse grained model termed Fermi-Jagla and 2) a more realistic q-tip4p/f model. A potential application of this water polymorphism to the cryopreservation of biomolecular systems will be discussed.

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