

Water in Hydrophobic Nanoconfinement

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Abstract:

Water is essential for the activity of proteins and cell function. However, the effect of the properties of water on the behavior of bio-macromolecules is only partially understood. Recently, several experiments have investigated the relation between thermodynamics and dynamics of protein hydration water and water under confinement. These works have generated a large amount of data whose interpretation is debated. Here we present recent results about theoretical predictions of a coarse-grained model of water hydrating hydrophobic interfaces. We consider different confining geometries and calculate how transport properties, such as the diffusion coefficient, dynamics quantities, such as the hydrogen bond relaxation time, and thermodynamics observables, such as compressibility, specific heat and thermal expansivity, change under confinement. We consider also the effect of water on protein stability, making a step in the direction of understanding how the interplay of water cooperativity and hydrogen bonds interfacial strengthening affects the protein cold denaturation.