

Interfacial water: from hydration repulsion to hydrophobic attraction

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Water plays an essential role in determining the interactions between biological molecules and inorganic materials. Hydrophilic surfaces in contact with water, such as DNA, charged membranes, or mineral surfaces, exhibit an unusual strong repulsion at very short distances (≈ 1 nm). Despite a significant number of experimental and theoretical studies, the physical origin of this repulsive force, *the hydration force*, is poorly understood, and the microscopic mechanism originating such force remains a controversial question in the modern theory of surface forces. On the other hand, hydrophobic surfaces in water experience very strong attractive interactions. This attractive interaction, *the hydrophobic force*, plays an important role in the self assembly of nano-materials and bio-molecules in solution. Hydrophobic forces between surfaces with dimensions larger than ≈ 1 nm, have been interpreted in terms of capillary forces, whose origin is the capillary evaporation of water confined between hydrophobic regions. Nevertheless, the theoretical models normally ignore the polarizable character of real hydrophobic substances. Recent experiments on inorganic materials and biomolecules, have challenged *drying* as the mechanism explaining the hydrophobic attraction.

I will discuss Molecular Dynamics computations of interfacial water at hydrophobic and hydrophilic surfaces. Firstly, current work on the interactions between polarizable hydrophobic solutes will be presented. I will show that a small degree of polarizability, similar to that expected in experimental systems, is enough to inhibit drying at the molecular scale. Weakly polarizable solutes can stabilise fluctuating reduced density regions between hydrophobic surfaces, which results in a strong attractive force. Our work suggests that drying might be an unlikely mechanism to explain hydrophobic attractions. Secondly, recent work on the origin of the hydration force will be presented. Large scale computer simulations of Newton Black Films have provided a detailed view of the structure and electrostatics of water at charged surfaces. We have found that water exhibits an anomalous dielectric response near these surfaces. This anomalous behaviour provides a microscopic mechanism to explain the hydration force.