

Water at Interfaces: Phase Transitions and Connection to Protein Dynamics

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Water is a unique liquid, many of its properties being critical for the continued support of life. In living systems, essential water-related phenomena occur in restricted geometries in cells and at active sites of proteins and membranes or at their surface. The effects of hydration on the equilibrium protein structure and dynamics are fundamental to the relationship between structure and biological function. In particular, the assessment of the perturbation of the structure and dynamics of liquid water by hydrophilic and hydrophobic molecular surfaces is fundamental to the understanding of the stability and enzymatic activity of globular proteins and functions of membranes [1].

Water plays a major role in the stability and catalytic function of proteins. Both the effect of hydration water on the dynamics of proteins [2,3] and the effect of proteins on the dynamics of water [4] have been studied using inelastic neutron scattering, the most direct probe of protein /water dynamics on the picosecond-nanosecond timescale. The peculiar structural and dynamic properties of interfacial water, in particular the phase transitions that interfacial water experiences at low temperature, will be presented. We will discuss: i) the connection between the interfacial water phase transitions and the dynamics of protein, ii) how the protein-hydration water interaction can drive the protein function [5].

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