

NEUTRON SPECTROSCOPIC STUDIES OF INTERACTION BETWEEN WATER AND DNA/PROTEINS AND AMINO ACIDS

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The interaction of water with proteins with respect to their structure and function is a recently emerging field. We have recently studied water dynamics in DNA, proteins and biopolymers using neutron spectroscopic techniques [1,2]. Our studies of water in DNA, proteins and biopolymers shed new light towards the understanding of the structure and dynamics of water in the biological environments. However, the complexity of proteins (consisting of hundreds of amino acids) has so far proven too difficult for us to make a more precise understanding of the relationship between the water structures of hydration sites on the biomolecules. In order to make further progress in this field, we have studied the systems of water and amino acids which is the basic building block of proteins (e.g. Glycine, Alanine, Glutamate and Serine) under different extreme conditions. These molecules exhibit the following properties, small, well characterised and having known interaction sites with water, these systems provide an excellent opportunity for us to study their hydration states. By comparing with the known states of water [3,4], the neutron scattering spectra show new insight towards our understanding of the interaction between water and the amino acids. Based on these spectra, we also performed ab initio simulations which would provide the necessary assignment for the vibrational modes seen in the measured INS spectra.

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