Neutron spectroscopy investigation of water and water in biomaterials

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The use of modern physical research tools to investigate biological systems (i.e. their structure and dynamics) is the main theme of biophysics. The recent advances in the high-flux and high-resolution synchrotron, neutron scattering facilities, high resolution of STM/AFM and compute simulation techniques developed initially by physicists, provide scope of possibilities to attack biological problems which were not possible before. In the recent years, some of our research effort has been gradually switched from pure water to water in biological systems using inelastic, quasi-elastic and neutron Compton scattering techniques, for instance looking at the structure of water inside and around DNA/protein molecules to see how they interact with water molecules, above all how water molecules interact among themselves under biological environments which has paid very little attention in the past. Using diffraction (X-ray or neutron) techniques is very difficulty for this type of study, because firstly, although (synchrotron) X-ray has a better resolution and luminosity, lack of ability to see protons makes it very unsuitable for examining the structures of water (the orientations of water molecules in particular). Neutron scattering, on the other hand, has the ability to see proton positions, however the complex structures of DNA and proteins and the arrangements of water molecules around make it very hard to gain a clear picture of the special arrangements, often averaged (time and molecule) positions are given. However, using neutron vibrational spectroscopy we can define the local structures of water molecules by comparing the vibrational signatures with known configurations in high-pressure phases of ice. The effectiveness of this method has been clearly demonstrated from our early work for the exotic phases of ice [1,2] and water in a range of porous systems [3]. The work shows the existence of two strengths of hydrogen bonding in water/ice [1] which would not only provide a mechanism for the explanation of the range of water anomalies, but it also indicates that water may have a very active role (like a catalyst) in the formation and stabilization of DNA, proteins and membranes. By adopting different water-water configurations in the protein structures, the interaction forces of the H-bonds can change very drastically up to 90% [4] and hence the vibrational frequencies will change and can be observed in the measured inelastic neutron scattering spectrum with very high accuracy even at very low concentrations of water present. This change of interaction as results of change in the local water structure will inevitably alter the structure and functionality of the biomolecules, answering many phenomena related to the protein folding which heavily relies on the H-bonding with surrounding water molecules. In the paper, we will present a series of neutron spectroscopic measurements for a range of proteins (e.g. photo system II and anti-freeze proteins), biopolymers and DNA materials using newly developed instruments such as TOSCA and HET in the energy transfer range from 2 to 500 meV (15 cm^{-1} to 4000 cm^{-1}).

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