UREA-WATER DYNAMICS IN PROTEINS: AN ULTRAFAST SPECTROSCOPIC STUDY

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Water plays a vital role in many biological processes like enzyme activity, protein folding-refolding and denaturation. It is essential to know the time scales characteristic of both, the local protein rearrangements and water dynamics within the solvation shell to understand the protein-water interactions. Urea is a chaotropic agent and a well-known denaturant for proteins. The molecular picture of the interaction of urea with the water hydrogen bond network and thereby, the chemical denaturation of the proteins is still ambiguous. Time-resolved Optical Kerr effect (OKE) spectroscopy is a powerful spectroscopic technique to study the hydrogen-bonded structure and dynamics of complex aqueous systems, in the picosecond time scales. In this study, we have investigated the mechanism behind urea denaturation of three proteins of different hydrophobicities- lysozyme, BSA and trypsin.

The OKE data reveals the effect that different concentrations of urea have on the aqueous protein solutions. The spectral density (SD) obtained contains the α relaxation at the lowest frequencies corresponding to the orientational diffusion of the molecules, linked by the stretched β relaxation to the intermolecular librational modes at terahertz frequencies. The shape of the SDs resembles that of urea solutions; the addition of protein brings down the contribution from the α relaxation. At lower urea concentrations, this change is even more apparent. Preliminary analysis of the SDs shows the β relaxation timescales of water changes on the addition of urea and the subtracted spectra for the urea denatured lysozyme shows two distinct β processes characteristic of water and water-urea dynamics. A detailed analysis of the changes in the line shapes of the reduced spectral densities (RSDs) is required to elucidate the effect urea has on the water hydrogen bond network and to map out the structural changes occurring in three different proteins on the addition of urea.