

Hydration of bio-molecules by combined use of synchrotron-based UV Resonance Raman and Neutron Scattering experiments

Water-protein interactions are thought to play an important role in determining protein structure and function. Yet, a complete microscopic description of the interactions between water atoms and specific sites of the peptide backbone and its side chains is still lacking. A description at the atomic scale of water hydration can provide insights on still open and important issues like protein folding and association as well as protein-ligand binding. We can tackle this issue by looking at the interaction between water and specific groups of small peptides. The biological activity of peptides is strictly connected to the solvent properties, which plays a fundamental role in driving their functions. Nevertheless and beside the biomedical relevance of these small bio-molecules, peptides can be still considered simple model systems to tackle water (or solvent)-protein interactions at the atomic scale. In particular, we would like to exploit synchrotron-based UV Resonance Raman and Neutron Scattering experiments for investigating the properties of the hydration shell around peptides at physiological conditions and in the presence of solvents made up by water and protic ionic liquids (IL). The rationale behind this approach is based on the key feature of ILs, namely their infinite range of the bare electrostatic interaction, which leads to Debye screening and charge ordering effects. In the present context, the possibility for a protic IL either to replace water or act as a co-solvent for biomolecules, has implications related to protein stability, folding, and catalytic activity. UV Resonance Raman (UVR) scattering is a powerful technique for providing molecular information on the solutions of bio-macromolecules, such as peptide and proteins. The use of a tunable deep UV Raman system (as implemented at the UVR setup working with the synchrotron radiation source available at Elettra Sincrotrone Trieste) allows for selective enhancement of different chromophores within the sample. In particular, by finely tuning the excitation wavelength used for collecting UVR spectra, it is possible to selectively enhance the Amide signals that, as known, are vibrational modes particularly diagnostic of the conformational changes occurring in peptide and proteins. The molecular information provided by UVR technique are complemented by the structural view offered by neutron diffraction experiments able to give an atomic length scale description of the peptide-water interaction at specific sites of biomolecules.

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