

IT IS WATER WHAT MATTERS: THz SPECTROSCOPY AS A TOOL TO STUDY HYDRATION DYNAMICS

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Terahertz absorption spectroscopy has turned out to be a new powerful tool to study biomolecular hydration. The development of THz technology helped to fill the experimental gap in this frequency range. These experimental advances had to go hand in hand with the development of theoretical concepts that have been developed in the recent years to describe the underlying solute-induced sub-picosecond dynamics of the hydration shell. This frequency range covers the rattling modes of the ion with its hydration cage and allowed to derive major conclusions on the molecular picture of ion hydration, a key issue in chemistry. By a combination of experiment and theory it is now possible to rigorously dissect the THz spectrum of a solvated biomolecule into the distinct solute, solvent and solute-solvent coupled contributions. Moreover, we highlight recent results that show the significance of hydrogen bond dynamics for molecular recognition. In all of these examples, a gradient of water motion toward functional sites of proteins is observed, the so-called hydration funnel. The efficiency of the coupling at THz frequencies is explained in terms of a two-tier (short- and long-range) solute-solvent interaction.