New Insights into the Role of Water in Biological Function: Terahertz Absorption Spectroscopy Studies of the Solvation Dynamics of Biomolecules

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In life science water is the ubiquitous solvent, sometimes even called the "matrix of life". There are more and more experimental and theoretical evidences that solvation water is not a passive spectator in biomolecular processes. We could show that THz absorption spectroscopy is a new tool to study the coupled protein solvation dynamics of biomolecules. Our studies revealed that an efficient dynamical coupling of the THz dynamics of biomolecules with those of their hydration shells can play a key role in biomolecular mechanisms.

The development of Kinetic THz Absorption (KITA) spectroscopy allows us to follow changes in hydration dynamics in real time during biological function. Using a combination of time resolved X-ray studies and THz absorption studies we find that, as enzyme–substrate binding develops, but before a full complex is formed, the movement of water near the protein is retarded. Crudely put, it is as if the water 'thickens' towards a more glassy form, which in turn calms the fluctuations of the substrate so that it can become locked securely in place.

A two-tier (short-range and long-range) solute-solvent interaction together with a heterogeneous hydration dynamics towards functional sites appears to be a fundamental element of molecular recognition. We propose that this gradient of water motions, the so-called "hydration funnel" is playing a -so far neglected- role. These results offer an astonishing picture of how finely biomolecules manipulate their associated water molecules to perform their function.