HYDRATION DYNAMICS OF BIOMOLECULES INVESTIGATED BY THZ SPECTROSCOPY

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Using our high-power p-doped germanium laser (2.4-2.9 THz, $\sim$ 1 watt average optical power) spectrometer in a double-beam configuration, we demonstrated that THz spectroscopy is a highly accurate tool to probe hydration dynamics of biomolecules. Recently, we extended our analysis to the five helix bundle protein lambda repressor and the highly conserved regulatory protein ubiquitin and found a strong nonlinear behavior of THz absorption as a function of protein concentration. We explain this behavior by coupling of the protein and the proteins hydration water layer network. A dynamic interplay between proteins and their hydration shells is observed on the picosecond and sub-picosecond timescale. The experimental data suggest an influence on the correlated water network motion beyond 20 Å, greater than the pure structural correlation length usually observed. Molecular dynamics (MD) simulations support our model and give a more detailed insight into the observed dynamics on a microscopic scale. The simulations indicate water dynamics in the hydration layer around one protein to be distinct from bulk water out to 10 Å.
Together with MD simulation, THz spectroscopy is a new, highly sensitive tool to analyze hydration water dynamics coupled to small biomolecules and proteins in their native environment.