It Is Water What Matters: THz Absorption Spectroscopy As A New Tool To Study Solvation Dynamics

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***Abstract*—Terahertz (THz) absorption spectroscopy is a powerful tool to study (bio)molecular hydration. The development of THz technology helped to full 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 so-called rattling modes of the ion with its hydration cage and allows to derive major conclusions on the molecular picture of ion hydration, a key issue in chemistry. THz spectroscopy allows the quantification of the hydration shell around ions, and the characterization ion pairs.

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".

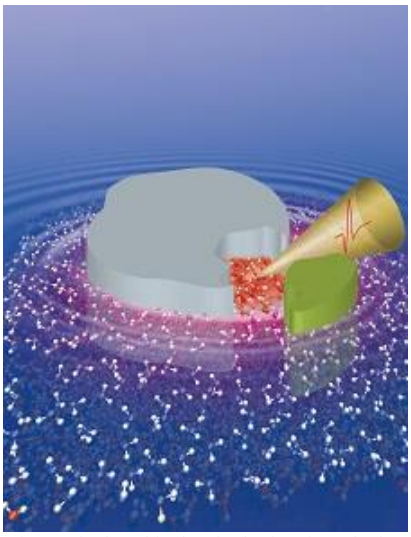

Fig 1. Displayed is the "hydration funnel", i.e. the site with retarded water dynamics at the active site. Collective hydration bond dynamics is probed with THz spectroscopy

REFERENCES

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