Keeping an eye on the surroundings

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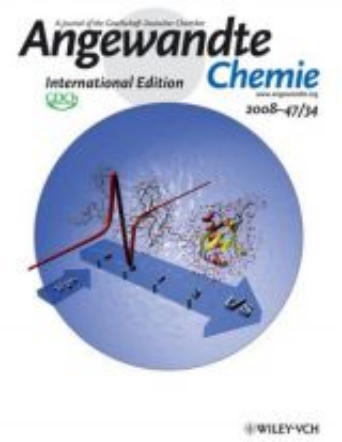

Kinetic terahertz absorption (KITA) uses a picosecond-duration terahertz pulse to monitor directly changes in solvent dynamics during molecular self-assembly on a reaction time scale of milliseconds to seconds. In their Communication, M. Gruebele and co-workers describe the application of this method to investigate the reorganization of solvent water during the folding of a protein (in this case ubiquitin). Credit: (C) Wiley-VCH 2008

Water is no passive spectator of biological processes; it is an active participant. Protein folding is thus a self-organized process in which the actions of the solvent play a key role. So far, the emphasis in studies of protein folding processes has been on observation of the protein backbone and its side chains. Researchers led by Martin Gruebele and Martina Havenith have now been able to detect changes in the protein–water network during protein folding in real time.

As they report in the journal *Angewandte Chemie,* this team of scientists at the University of Illinois (Urbana, USA) and the Ruhr University in Bochum (Germany) used a spectroscopic technique called KITA (kinetic terahertz absorption) to make their observations.

Terahertz (THz) radiation consists of electromagnetic waves in the submillimeter range, putting it between the infrared and microwave ranges. Efficient sources of THz radiation are now available, making it possible to directly measure the absorption of biomolecules in aqueous buffers on the picosecond time scale. Both the skeletal movements of proteins and the collective motions of water molecules surrounding proteins occur on this time scale.

The research team recently demonstrated that THz-range absorption spectroscopy is a sensitive method for the investigation of the water shell that surrounds proteins. In the layers immediately surrounding the protein, the water molecules are networked to each other differently than in pure water. Their absorption of THz radiation at certain frequencies is thus changed.

The way in which a protein folds to a very large extent determines its function. The folding process is very fast. The movements of the protein backbone influence the solvent, and the dynamics of the solvent can in turn influence the dynamics of the protein—thus playing an important role in the folding process. Kinetic THz absorption (KITA) registers the damping and phase-shifting of an electrical THz field caused by the folding of a protein. Comparison with results obtained by other methods confirms that KITA detects reorientations of the interactions between a protein and its water shell in an early phase of the folding process.

Source: Wiley