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Arnimallee 14

Vorstellungsvortrag zur Habilitation

Am Dienstag, den 22. Januar 2002, 16 h c.t.

spricht Dr. Erik Nibbering

MBI

über Strukturelle Dynamik auf ultrakurzen Zeitskalen –
Femtosekunden Schwingungsspektroskopie
als experimentelle Methode

Due to recent improvements in ultrafast mid-infrared technology it is now apparent that the following major advantages can be denoted of femtosecond mid-infrared spectroscopy that enable detailed structural dynamical information on molecular geometries and interactions. For instance, the (time-dependent) spectral position and band shape of a "spectator"-mode gives dynamical information of chemical bonds. Comparison of experimental vibrational patterns with quantum chemical calculations lead to determination of geometric structures of transient states. Direct geometric information can be obtained from pump-probe experiments on vibrational bands that exhibit features of anharmonic coupling between vibrational modes.

In this seminar I demonstrate this progress by highlighting some of our studies at the Max Born Institut on the ultrafast structural dynamics of hydrogen bonding interactions. Hydrogen bonds are an important type of local interaction in which a hydrogen atom is shared by donor and acceptor groups. Such bonds play for instance a fundamental role for the three-dimensional structure and dynamics of protic solvents such as water, and of biomolecular systems such as proteins and DNA. Dynamics of hydrogen bonds occur on ultrafast time scales set by vibrational motions of hydrogen donor and acceptor groups and are not well understood on a microscopic level. Several key experiments demonstrate the potential of elucidating the structure and dynamics of hydrogen bonds of molecular complexes after electronic excitation.