Two-dimensional infrared spectroscopy: a new tool to study complex molecular systems

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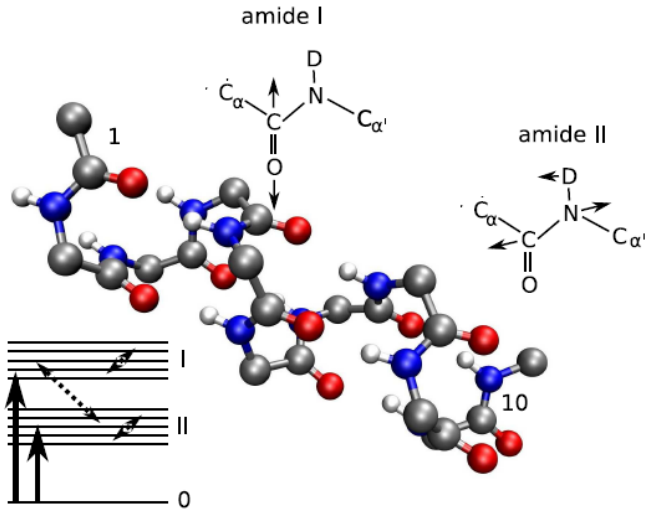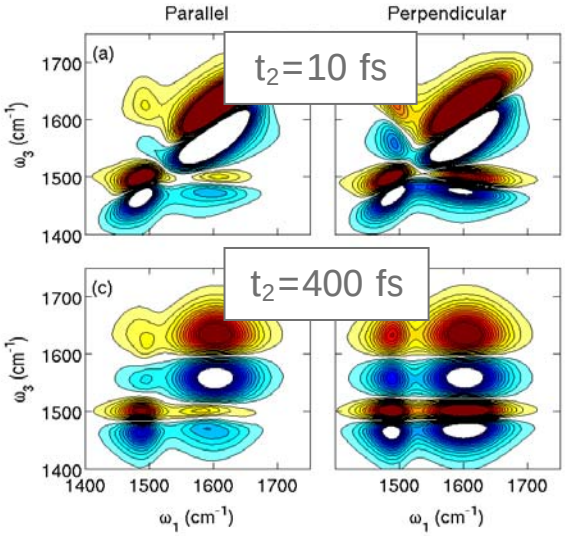
Two-dimensional infrared spectroscopy (2DIR) is a tool developed during the past decade to study structural and dynamical properties of complex molecular systems, such as proteins and DNA. In analogy to two-dimensional NMR, 2DIR probes temporal and spatial correlations between vibrational transitions. As vibrational frequencies depend on molecular conformation and properties such as hydrogen bonding, the technique is sensitive to molecular structure. With the use of femtosecond infrared pulses, ultrafast structural and excited state dynamics may be resolved. As 2DIR spectra have complex and often convoluted lineshapes, their interpretation requires novel modelling techniques that enable one to describe the vibrational couplings and dynamics in detail. In this seminar I will introduce the experimental method and discuss our computational tools developed during the past years to unravel existing experiments and to suggest new ones. I will discuss applications of our method to peptides and small proteins in solution and to the problem of proton transfer in a transmembrane channel.