From ultrafast structure determination to controlling photochemistry:

2D-IR spectroscopy in chemistry and biophysics

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Resolving structure and dynamics of short lived molecular species is the key to (bio-)molecular function and reaction mechanisms. To access these structures, a method combining structure resolution and high time resolution is required. Ultrafast two-dimensional infrared (2D-IR) spectroscopy is an excellent complement to commonly used methods such as NMR spectroscopy in the presence of fast chemical exchange and for investigating short lived species. Different 2D-IR experiments have been implemented that measure energy transfer,[1] couplings[2,3] and correlations[4] of vibrations, which reveal molecular structure and its change in time. Combination with unnatural amino acids allows for novel insights into protein dynamics.

The use of mixed IR/VIS techniques further extends the application range of 2D-IR spectroscopy,[5] enabling studies of ultrafast light triggered processes,[4] subensemble-selective photochemistry[6] as well as surface specific,[7] highly sensitive experiments.

In my talk I will illustrate the utility of different 1D and 2D-IR experiments, using examples from enantioselective catalysis, photochemistry, electrochemistry and protein biophysics.

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