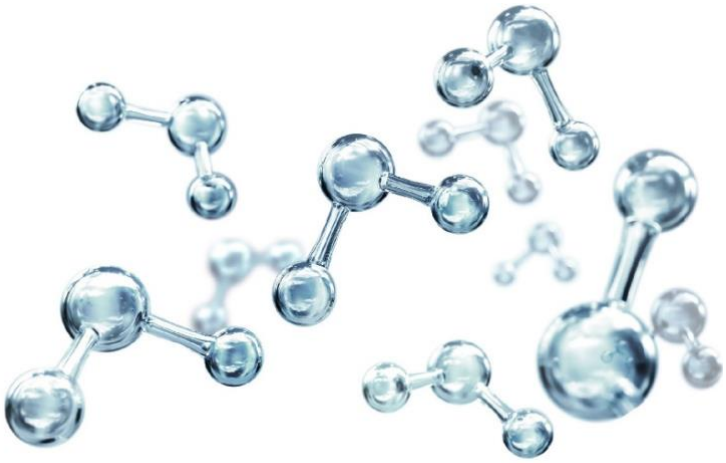
Seminar

CMWS Centre for Molecular Water Science

19th of May 2022
12:00 h

Zoom Virtual Meeting:

https://desy.zoom.us/j/84703564086
Meeting-ID: 847 0356 4086
Password: 570173



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Mapping Energy Landscape of a Hydrogen-Mediated Chemical Bond with Femtosecond 2D Full Mid-IR Spectroscopy

Short strong hydrogen bonds (SHBs) are present ubiquitously in biomolecules, around strongly polarizing ions in water, in fuel cells, atmospheric aerosols and interstellar space. They were hypothesized to play an important role in enzymatic catalysis, allosteric pathways and signal transduction, proton transport and ion hydration. Direct experimental investigation of their properties is often hindered by the data complexity, ambiguity of their interpretation and overlapping contributions of other molecular constituents. On the theory side, strong couplings render the problem intractable for standard quantum chemistry calculations. As a result, not only these bonds remain poorly characterized, but various reports outright deny their functional relevance. Ultrafast 2D IR spectroscopy is a powerful tool to characterize the anharmonic vibrational potentials of hydrogen bonds. Typically, 2D IR spectra cover at most 250×250 cm^{-1} spectral regions, thus only encompassing several vibrational bands. Here I will discuss the first 2D full mid-IR spectrum of an aqueous SHB where both axes span the entire 1000-4000 cm^{-1} mid-IR range. It allows to comprehensively map the energy landscape of a typical SHB and in conjunction with the state-of-the-art multidimensional anharmonic quantum chemistry calculations to reveal the counterintuitive spectroscopic and energetic properties of this bond.