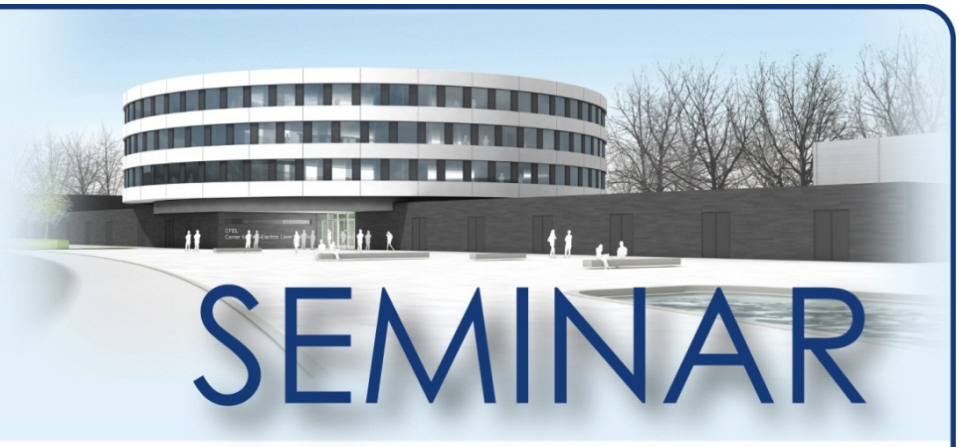
CFEL SCIENCE



SEMINAR

13th December 2023 - 2:00 p.m.

CFEL-bldg. 99, seminar room IV

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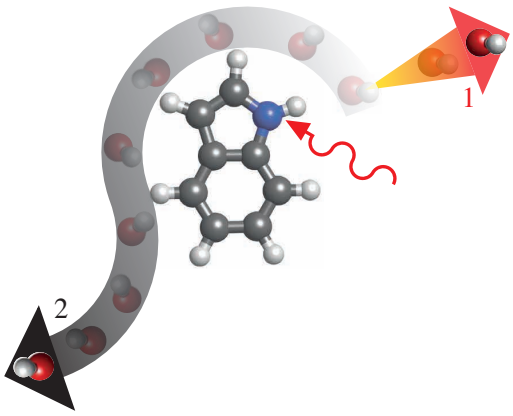
Initiating and unravelling gas-phase thermal-energy dynamics

“Everyday chemical processes”, from biological to industrial, typically occur at thermal energies, i.e., excitations that best correspond to the energy of mid-infrared (mid-IR) photons. While the dynamics of numerous gas-phase molecules have been tracked following electronic excitation by visible, ultraviolet or x-ray photons, few experiments have used mid-IR triggers. This is mostly due to “THz-gap” challenge, i.e., the difficultly of creating suitably bright ultrashort mid-IR laser pulses for initiating thermal-energy dynamics in gas-phase systems. Yet, with the advent of advanced optical parametric amplifiers, we propose that this challenge has been overcome, and ultrafast dynamics of gas-phase systems can be studied not simply in the near future, but today [1].

To demonstrate these possibilities, I present our recent efforts to trigger and track the thermal-energy-induced dynamics of indole-water—a micro-solvated model system for studying the interactions between proteins and their environment, with the water molecule locally bound at the N-H bond of indole. With a suitable sample created via supersonic expansion and the use of an electrostatic deflector, a tuneable ultrashort mid-IR laser pulse, with its wavelength set to ~2900 nm to match the N-H vibrational excitation of indole-water, is used to trigger the reaction—with this process characterised in the accompanying figure. Probed via strong-field-ionisation ion-mass-spectrometry methods, results indicate that the cluster dissociates after excitation, and that efficiency of excitation is sensitive to the overlap between the absorption band and the laser spectrum.



This work is the first step towards building a picture of ultrafast thermal-energy dynamics of gas-phase systems using femtochemistry methods.

[1] Robinson & Küpper, Phys. Chem. Chem. Phys. (2023), published online: 10.1039/D3CP03954D, arXiv:2308.09602

Host: Robin Santra – CFEL-DESY Theory Division