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 CFEL-bldg. 99, seminar room IV

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Ultrafast energy transfer from solvent to solute induced by sub-ps highly intense THz pulses

Temperature-jump (T-jump) experiments have a long history in the study of chemical kinetics. With the advent of femtosecond lasers a couple of decades ago, ultrafast T-jump experiments became possible and have since been used to study the very fast kinetics of fundamental steps in chemical reactions, folding processes in biomolecules and fundamental aspects of the hydrogen bond dynamics and energy transfer in liquid water and other liquids. T-jumps in water can be induced e.g. by targeting the first O-H vibrational excitation of liquid water at about 3400 cm^{-1} with an infrared (IR) laser, thus providing T-jumps in the nanosecond to femtosecond timescales. Till now, the T-jump in liquid water is limited only to the order of few tens of K with IR pump. Such temperature jump is very small in comparison to the thermal energy $k_B T$ associated with typical chemical reaction barriers in solution.

I will talk about the response of liquid water to one and half cycle, 141 fs long (FWHM) THz pulses spectrally centered at about 100 cm^{-1} (3 THz). At low intensity, THz light couples to low energy collective modes of the liquid. But the H-bond network among water molecules can't be reduced significantly by until the intensity of the pulse is higher than a minimum intensity. The pulse with an intensity of about $5 \times 10^{12}\text{ W/cm}^2$ transfers the energy mostly to the translational and rotational modes of the water monomers in a small time-scale. Water reaches to a state which is gas like very hot liquid. I will also discuss the response of solute (phenol as an example) to such THz pulse in the aqueous solvent. The phenol in liquid water gains significant amount of energy due to strong collision of highly mobile water molecule. This study implies that the energy supplied by the THz can potentially activate chemical processes long before the large amount of energy supplied leads to volume increase and vaporization of the medium.

Fig: Kinetic Temperature (T_k) of water and the dissolved phenol molecule.

