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Ultrafast Energy Transfer to Liquid Water by Short and Intense THz Pulses

Liquid water is the single most important medium in which chemical and biological processes take place. Rather than acting as passive environment, the dynamics of water during chemical and biological processes play a fundamental role in the solvation and stabilization of reaction intermediate. The possibility to generate sub-ps and very intense THz pulses at free-electron lasers in full synchronization with the X-rays (XFEL) opens the possibility to time-resolved investigations of transient state of water and of molecular species dissolved in it. Liquid water has been the subject of time-resolved X-Ray spectroscopy studies at XFELs in the past. It's response to intense pulse in the infrared domain, in which mostly intramolecular vibrations are excited, and the subsequent energy dissipation processes, have been extensively studied in the past. At low frequency, THz light couples to low energy collective modes of the liquid.

Here, we investigated the response of liquid water to one-cycle,200fs long THz pulses spectrally centered at about 100/cm (~3THz). The THz pulse does not target any particular mode of the liquid. At an intensity of about 10^(10) W/cm^(-2), the pulse transfers energy mostly to translational modes of the water monomers along the polarization axis of the electric field. In a time-scale of 500fs to 1ps the energy redistributes to hindered rotational modes first, and to intramolecular vibrations last. This 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. Radial Distribution function and X-Ray diffraction pattern of water at certain time intervals are showing that water looses tetrahedral hydrogen bond structure with time due to pulse. Water reaches to a quasi-equilibrium state which is gas like very hot liquid. In this study, we have used CP2K package for Ab-Initio Molecular Dynamics.

We are also investigating the energy gain by Phenol molecule in an environment of liquid water by THz pulse.

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