Electron Dynamics After Strong Field Ionization of Liquid Water

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The transport and solvation dynamic of charge carrier in water plays a key role in understanding the destruction mechanism of biorelevant molecules. The relaxation dynamics of the highly reactive photoproducts formed during strong field excitation of liquid water are investigated by polarization and phase-sensitive transient absorption spectroscopy with few-cycle pulses. In addition, the phase change anisotropy signal around delay time zero is analyzed by sliding window Fourier transform method and correlated to beyond Born-Oppenheimer dynamics of short-lived water ions. To our knowledge, this is the first experimental observation of this kind of nuclear dynamics in the context of pump-probe experiments.

Our data indicate that upon strong field excitation by CEP-stable pulses, the water molecules are ionized and generate free electrons and holes. Within our beyond Born-Oppenheimer dynamics studies, the reduction of H_2O^+ with a simultaneous increase of $H_4O_2{}^+$ can be observed with a time constant of 18 fs, as a transition state within H_3O^+ and OH formation. In contrast, the electron can be given as quasi-free within the water conduction band within the first 100 fs. The excess energy of these "hot electrons" is transferred to the water environment by inelastic scattering and the electrons thermalize towards the conduction band minimum. At this point, the representation of liquid water as an amorphous semiconductor breaks down and the water-specific localization path comes into play. The thermalized electrons can be trapped in shallow "wet" states created by weak or broken hydrogen bonds. The surrounding water molecules begin to optimize their position and orientation due to dipole interactions, leading to a further reduction in the potential energy of the trapped electrons.