Simulation for electron dynamics in solid under intense laser pulse

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We have been developing a real-time, real-space computational method to describe electron dynamics based on the time-dependent density-functional theory (TDDFT). This method has been successful to describe linear optical responses of molecules and solids [1]. We are currently applying the method for nonlinear and nonperturbative dynamics of electrons in molecule and solids induced by intense, ultra-short laser pulse.

When the strength of the electric field of laser pulse is comparable to the electric field which binds electrons in materials, a variety of phenomena reflecting nonlinear electron dynamics are observed. They include multiphoton and tunnel ionizations, rescattering phenomena which induce high harmonic generation in atoms and molecules, and optical breakdown in dielectric materials. In my presentation, I would like to discuss our recent study on nonlinear electron dynamics induced by intense laser pulse, mainly in solid, employing the real-time, real-space implementation of the TDDFT.

Our basic equation to describe electron dynamics in solid is the time-dependent Kohn-Sham equation in which the induced polarization field as well as the external laser electric field are treated as the time-varying, spatially uniform vector potential, taking long-wavelength limit. The time-evolution of the induced vector potential is determined by the current averaged over the unit cell. When this framework is used for a weak external field, the Fourier decomposition of the induced vector potential gives us frequency-dependent dielectric function [2].

We will show our calculations for diamond, a typical dielectric material. We observe that the calculated results show the dielectric breakdown when the laser intensity approaches 10^{15}W/cm^2 where the laser electric field is comparable to the electric field acting on valence electrons. We discuss in detail an interesting nonlinear dynamics described by the time-dependent Kohn-Sham scheme which induce the optical dielectric breakdown.

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