

Ab-initio description for laser-induced electron-phonon dynamics in dielectrics

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We have been developing a theoretical and computational approach describing electron-phonon dynamics in bulk material induced by intense and ultrashort laser pulses. Our approach relies upon the time-dependent density functional theory, a successful first-principles theory for electronic excitations. We solve the time-dependent Kohn-Sham equation in real-time and real-space. The electron dynamics can be visualized in femtosecond time scale, which helps much to get an intuitive understanding for the dynamics. The following figure shows a snapshot of electron dynamics in bulk Si induced by an ultrashort laser pulse.

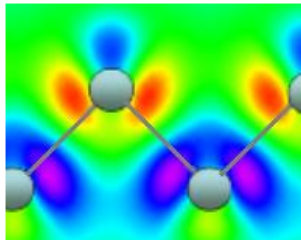


Figure 1: A snapshot of photoinduced electron dynamics in bulk Si.

We have applied our theory for several processes and have found that it provides a unified and quantitative description for the electron-phonon dynamics in femtosecond time scale. Under an intense laser pulse, it can describe optical breakdown of dielectrics induced by nonlinear ionization processes [1]. For a moderate intensity pulse, a coherent optical phonon generation can be described [2]. We have confirmed that our theory is capable of describing two distinct mechanisms, the impulsive Raman scattering and the displacive excitation, in a unified way.

[1] T. Otobe et al, Phys. Rev. B **77**, 165104 (2008); J. Phys. Cond. Matter **21**, 064224 (2009).

[2] Y. Shinohara et al, J. Phys. Cond. Matter, in press.