

Observables of real-time lattice dynamics in time-dependent density functional theory

I will discuss real-time simulations of lattice vibrations in solids and their signatures in spectroscopy. In particular signatures of electron phonon coupling in optical and electron spectroscopies have long been used to investigate materials. With the increasing interest in controlling and manipulating materials properties in a non-equilibrium state, such signatures become relevant also in time-resolved measurements. I will discuss how real-time time-dependent density functional calculations can be used to understand spectral features of electron-phonon coupling of driven electronic structure in solids. A useful interpretative tool that emerges from such a treatment is the picture of a dressed electronic structure, which allows to discuss effects in driven systems without referring to perturbation theory.