Theoretical description of laser induced ultrafast structural changes in condensed matter

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The interaction of femtosecond lasers with materials gives rise to a variety of interesting ultrafast phase transitions. Ultrashort light pulses usually act on times scales comparable to those characteristic for the motion of ions in solids, and create an extreme nonequilibrium state in which the temperature of the electrons and that of the ionic degrees of freedom differ by many orders of magnitude. As a consequence, ultrafast self-organization processes involving collective (and sometimes also coherent) motion of the ions are initiated.

In this talk we will first present a general theoretical framework for the description of laser induced structural changes in condensed matter[1,2]. Within this theory, different techniques can be used, like (i) molecular dynamics simulations on the basis of time-dependent potential surfaces, which are obtained from microscopic Hamiltonians and include explicitly the laser pulse[2], and (ii) construction of accurate laser excited potential energy surfaces obtained from all-electron density functional calculations.

In the framework of this approach the following problems will be addressed:

- Laser manipulation of carbon nanostructures and solids[3]
- Laser excitation of coherent phonons in Bi [4]
- Nonthermal melting of semiconductors (Si,InSb, Ge)[1,6]
- Laser induced “undoing” of a Peierls distortion in As[7]

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