ensity Functional Theory Beyond the Born−Oppenheimer Approxi

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Density Functional Theory Beyond the Born−Oppenheimer Approximation

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Traditional density functional theory, by its very nature, always involves the Born−Oppenheimer approximation: One calculates the electronic ground−state density corresponding to the electrostatic potential generated by clamped nuclei. In this lecture it will be outlined how one can go beyond the Born−Oppenheimer approximation by treating the fully coupled system of electrons and nuclei in terms of a multi−component density functional theory. Two different situations where the coupling between electronic and nuclear motion is important will be discussed in detail: (i) the superconducting phase of matter and (ii) the disintegration of matter in strong laser pulses.

Superconductors in thermal equilibrium are described in terms of three ``densities": The electronic density, the superconducting order parameter and a suitably chosen nuclear density. These quantities are determined by a set of Kohn−Sham equations which incorporate both normal and superconducting exchange−correlation (xc) effects. Approximate xc functionals describing purely electronic correlations in the superconducting phase, as well as xc functionals incorporating the electron−phonon coupling will be constructed and numerical predictions for T_c and other material−specific porperties will be presented.

A time−dependent multi−component density functional theory will be developed to treat matter in strong laser pulses. Approximate time−dependent xc functionals will be presented and dissociation processes such as the ionization−induced Coulomb explosion will be calculated.
