DFT Based Simulations of Electron Dynamics in Solids and Nanostructures

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We have recently used simulations based on time-dependent density functional theory (TDDFT) to study a number of problems related to the dynamics of electrons in solids and nanostructures. Some of the simulations are based on a simplified jellium description of large clusters, while in other cases the full complexity of the atomic structure is taken into account.

For example, the electronic energy loss of ions, like protons, antiprotons and He, has been studied in metals and insulators [1,2,3]. Although radiation damage processes are of extraordinary fundamental and technological importance, ab initio simulations of these effects in solids are still very scarce to date. Most simulations for solids and condensed systems are based on semi-empirical approaches, in which the effect of electronic stopping is frequently incorporated in simulations through an ion and target dependent friction coefficient. However, it has been recently observed that there are significant deviations from linearity at low velocities in insulators and noble metals, both showing different kinds of threshold effects. Our simulations using time-evolving TD-DFT could reproduce the anomalies in the stopping power observed experimentally for projectile velocities below 0.3 a.u., for insulators and noble metals [1,2]. We could also study the influence of the electron excitations on the effective internuclear forces when an Al target is bombarded with protons [3]. Understanding of such effects demands an explicit treatment of the electronic stopping in the presence of the actual atoms and actual electronic structure of the host system. For this reason, we have recently developed a version of the SIESTA code [4], a first-principles code that uses a linear combination of atomic orbitals as a basis set, that allows performing coupled electron-nuclear dynamics within the Ehrenfest approximation.

We have also considered the problem of the stopping of a particle nearby a metal surface, and whether it can be described using an effective, velocity independent, friction coefficient. For these simulations we have used jellium clusters of different sizes [5].

Time permitting I will comment on the methods that we have developed to estimate resonant charge-transfer times from adsorbates on metal surfaces using first-principles density functional calculations and some of its applications [6,7,8].

References

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