Keynote

Simulations of Electron Dynamics in Solids and Nanostructures with SIESTA

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We have recently used time-dependent density functional theory (TDDFT) to study a number of problems related to the dynamics of electrons and the optical response of solids and nanostructures. Our simulations are based on either real-time time-dependent SIESTA simulations or linear response calculations on the frequency domain.

To perform real-time time-dependent simulations we have developed a new version of the SIESTA code [1], 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. With this program we have studied the problem of the electronic energy loss of ions, like protons, antiprotons and He, in metals and insulators [2,3,4]. 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 [2,3]. 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.

We have also used linear response TD-LDA simulations to study the optical properties of large nanostructures. These simulations are performed using an efficient method developed by P. Koval et al. [5] that uses SIESTA ground-state simulations as a starting point. With an improved version of this method it has been possible to study the optical response of graphene quantum-dots with up to 1000 atoms (see Figure 1) [6,7], as well as to study the plasmonic resonances of large metal clusters.

References

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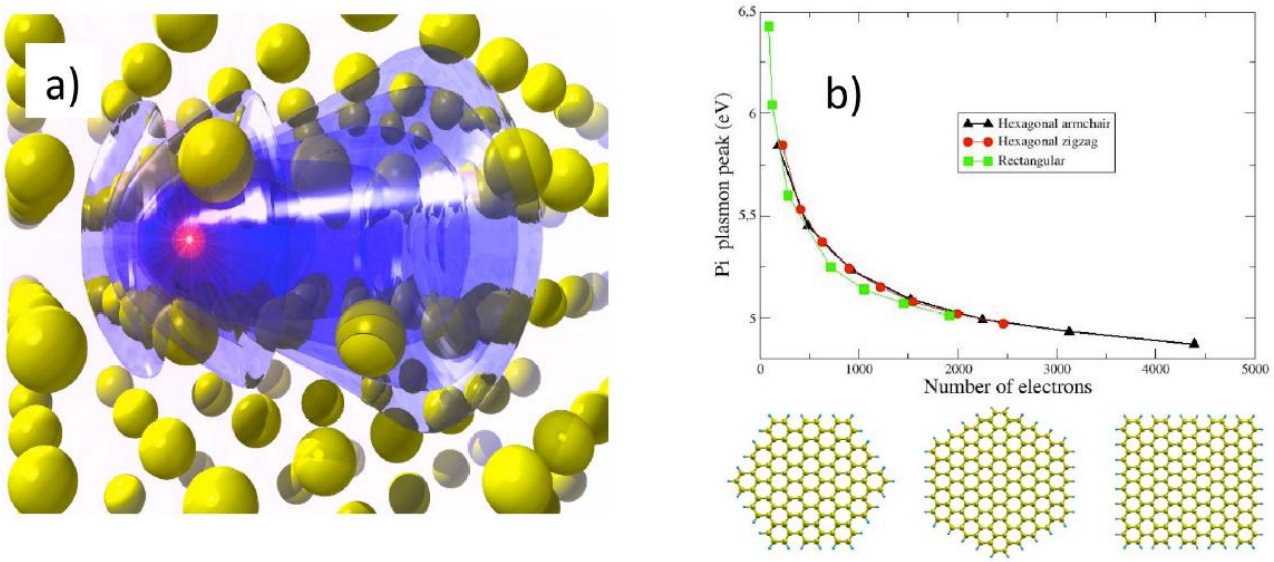

Figure 1. a) Isosurface of the induced density for a proton traversing an Al sample at v=0.5 a.u. (image by Alfredo Correa) [4]; b) Scaling of the main π-plasmon resonance for un-doped graphene quantum-dots of different shapes and sizes [7].