Ab-initio calculations of stopping power in solids

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Synopsis From the early models of electronic stopping power to the current first principles simulations, the techniques evolved to increase the range of validity and to reduce empiricism. Thanks to a combination of theoretical advances provided by Time Dependent Density Functional Theory (TDDFT) and the development of numerical codes, it became possible to predict electronic stopping power and evaluate energy losses in a variety of collision phenomena, including for realistic materials by performing direct simulations of the electron excitation processes beyond linear response, and including electronic band structure effects in solids.

Stopping power is a measure of the ability of a material to slow down energetic particles that travel in its interior. Given a certain type of energetic particle and a target material, stopping power is the amount of kinetic energy lost in relation to the thickness of material traveled. Stopping power is an important quantity used to predict and understand the effects of particle radiation in matter, ion ranges, the energy deposited, and ultimately the damage produced by energetic particles in diverse contexts, such as nuclear technology and medicine. The phenomenon of stopping power also gives us a glimpse on how matter reacts far from equilibrium, and in particular on the nature of the dynamic interaction between ions and electrons.

The microscopic processes that produce electronic stopping power are fundamentally dynamical and massively out-of-equilibrium. When the material is seen as a whole, the number of electronic excitations accumulate as the projectile moves, and multiple electrons are excited in the process. At the same time, electronic stopping power is a many-body problem, since the excitations are not produced and do not propagate independently.

For these reasons, the calculation of electronic stopping power in materials calls for explicit time-dependent simulation methods, as it would be very cumbersome to treat this problem by time-independent or systematically perturbative methods. This time-dependent strategy is analogous to the use of molecular dynamics in the classical theory of atoms and molecules. Specifically, Density Functional Theory (DFT) is a formal way to recast the many-body problem in terms of an equation for the one-body probability density. DFT inspired a family of useful approximations to model materials at the atomic and electronic levels; and it has been formally extended to time-dependent dynamics.

We employed real-time time-dependent density functional (TDDFT) dynamics with moving ions [1] to obtain electronic stopping at low velocity for protons, alpha and heavier ions in bulk systems, metals and insulator. In this talk we present several prototypical cases were first principles techniques are fundamental to describe the electronic stopping process and give a complete description of dissipative dynamics [2].

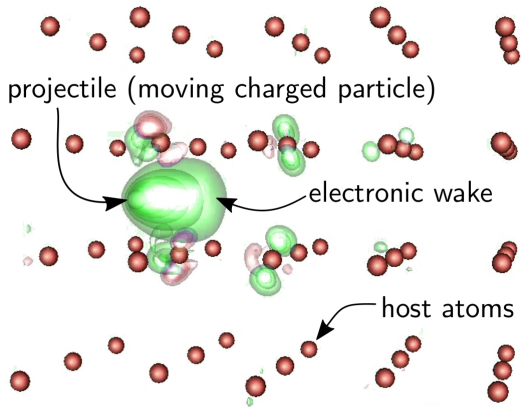

Figure 1. Density change differences produced by a H + moving in Cu atoms with $v = 1.8$ a.u. (81 keV) along the ⟨100⟩ channeling trajectory. [3]

References

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