Electron excitation in the nanoscale by ion projectiles shooting through matter

Emilio Artacho

Nanogune and DIPC, Tolosa Hiribidea 76, 20018 San Sebastian, Spain
Ikerbasque, 48013 Bilbao, Spain
Cavendish Laboratory, University of Cambridge, J J Thomson Avenue, Cambridge CB3 0HE, UK

e.artacho@nanogune.eu

Radiation damage of matter has been a topic of both fundamental and applied interest for over a century, from the nuclear industry to the treatment of cancer. Ion projectiles induce heavily non-equilibrium processes in the nanoscale, affecting the dynamics of nuclei and electrons [1]. Electronic stopping processes have been studied under two key paradigms, namely, linear response, for weakly non-equilibrium processes, and jellium host, for hosts close to ideal metals (see refs. in [1]).

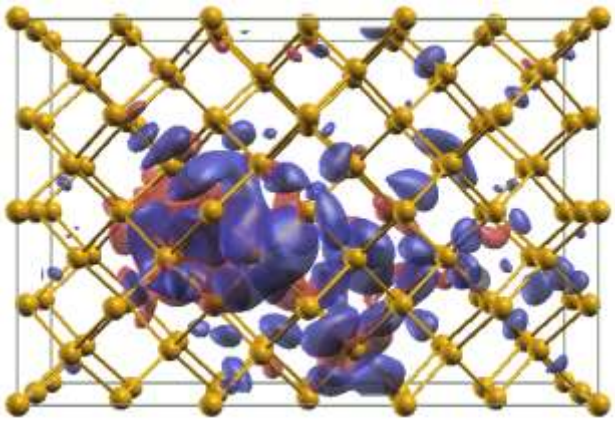

Figure 1: Dynamical deformation of the electron density by a passing proton [4], horizontally along the central axis of the box, right to left, v = 0.7 at. units. The proton is 70% across the box.

Recently, direct first-principles simulations were proposed for electronic stopping processes using real-time time-dependent density-functional theory, TDDFT(t), starting with the study of the threshold effect for protons and antiprotons shooting through a large-band-gap prototypical insulator [2]. The simulations consist of putting an ion in a large simulation box, set it in motion, and follow the TDDFT evolution of the electrons. Several approximations are involved, but it allows for arbitrarily strong non-equilibrium dynamical processes, and for any kind of host, as already successfully shown for noble metals [3], semiconductors [4], transition metals [5], in addition to the said insulators. In addition to results on electronic stopping processes, theoretical advances will be described that were prompted by this line of research. In particular, a differential geometry framework for expressing the TDDFT theory when using moving basis sets [6] and a Floquet theory for the characterisation of the stroboscopically stationary wave-functions for a constant-velocity projectile in a crystal [7]. Simulations of radiation-damage processes in nanosystems include electronic stopping in the nanostructured photovoltaic cells used in space, the study of electronic and electron-phonon processes in nanowires used for radiation resistant nanofoams [8], and chemical processes in carbon-ion chemotherapy [9].

References

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