

Electron excitation in the nanoscale by ion projectiles shooting through matter

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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]).

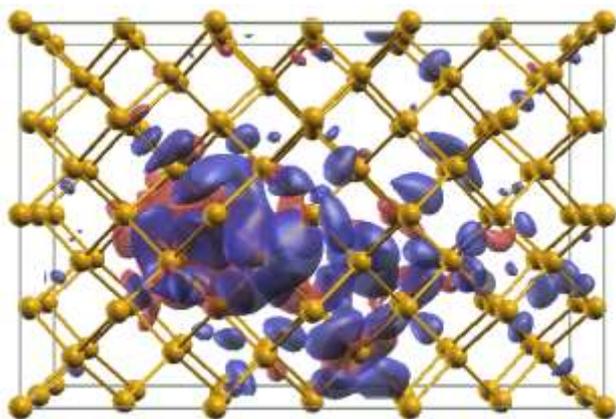


Figure 1: Dynamical deformation of the electron density by a passing proton [4], horizontally along the central axis of the box, right to left, $v = 0.7$ at. units. The proton is 70% across the box.

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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