Electronic stopping power for nuclei traversing matter from real-time time-dependent density-functional theory

Emilio Artacho [a,b,c]

[a] *CIC Nanogune and DIPC, Tolosa Hiribidea 76, 20018 San Sebastian, Spain.* [a] *Ikerbasque, Basque Foundation for Science, Bilbao 48011 Bilbao, Spain.*

[a] *Theory of Condensed Matter, Cavendish Laboratory, University of Cambridge, UK.*

email:

The study of particles (mostly nuclei) shooting through matter has a long history and is of relevance to understand radiation damage in important applied contexts, such as nuclear engineering, space, and radiotherapy. From the basic viewpoint radiation-damage processes are important as paradigmatic problems in the physics far from equilibrium. For projectiles with initial velocities around 0.2 a.u. or more the projectile slows down mostly by exciting the electrons of the target. Among the several models, theories and first-principles techniques to study electronic stopping processes, in 2007 we started a line of research based on the computational replication of those processes from first principles: In a simulation box of around 100-1000 atoms we put a projectile somewhere and start moving it across the box while the wave-functions evolve, within the framework of real-time time-dependent density-functional theory. The method involves many approximations, from technical to fundamental, but it has shown to be usefully accurate in its prediction of electronic stopping power at least in some cases. In this talk I will introduce the method, illustrate it with prototypical results, discuss some theoretical considerations around it, and present the latest results in the context of better understanding low-velocity threshold and Barkas effects in insulators and our still insufficient progress in addressing electron projectiles, of great relevance in radiotherapy.