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First-principles calculation of electronic stopping power in metals and insulators via time-dependent DFT simulations

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Projectiles interacting with solid or liquid targets are subject to two main inelastic collision channels: electronic and nuclear. The end result is a slowing down – or stopping – of the projectile due to energy deposition onto electronic excitations or motion of the target nuclei. At high projectile velocities, cross sections for nuclear stopping are exceedingly small, thus leaving electronic stopping as the only relevant channel. At low velocities nuclear stopping becomes predominant. In metals, it coexists with electronic stopping, but in insulators the existence of an energy gap for electronic excitations translates into a velocity threshold for electronic stopping. In this presentation I will introduce a recently developed computational methodology designed to study electronic stopping at the first-principles level, by means of time-dependent density-functional (TDDFT) simulations. I will then discuss the results for a variety of systems, starting from the first application to the ionic crystal LiF, moving to metallic systems like Al and Au, and then to the insulating water ice. In all cases I will compare to available experimental data to emphasize the astonishing accuracy of TDDFT results. I will also discuss how these simulations provide further insight into open questions such as the difference in stopping between H and He projectiles, and I will focus on the interplay between electronic excitations and non-adiabatic forces on the nuclei. Finally, I will touch on computational methods to simulate the combined dynamics of nuclei and electrons.

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