Accurate atomistic first-principles calculations of electronic stopping

Alfredo Correa
Lawrence Livermore National Laboratory

We show that atomistic first-principles calculations based on real-time propagation within time-dependent density functional theory are capable of accurately describing electronic stopping of light projectile atoms in metal hosts over a wide range of projectile velocities in the atomic unit scale. In particular, we employ a plane-wave pseudopotential scheme to solve time-dependent Kohn-Sham equations for representative systems of H and He projectiles in crystalline host materials.

This integrated approach to simulate non-adiabatic electron-ion interaction provides an accurate framework that allows for quantitative comparison with experiment without introducing ad-hoc parameters such as effective charges or assumptions about the dielectric function. This work shows that it is indeed possible to obtain a unified atomistic description of electronic stopping and that first-principles theory is able to capture the relevant physics, e.g. disentangle contributions of semi-core electrons and geometric aspects of the stopping geometry (channeling vs. off-channeling) in a wide range of velocities.

Applying the new implementation to systems with hundreds of atoms and thousands of electrons, we achieved excellent scalability on a large number of computer nodes (up to 1 million). Prepared by LLNL under Contract DE-AC52-07NA27344.