

Abstract Submitted
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First-principles calculation of electronic stopping contributions from core electrons and off-channeling¹ ALFREDO CORREA, ANDRE SCHLEIFE, Lawrence Livermore National Laboratory, YOSUKE KANAI, University of North Carolina, Chapel Hill — In order to understand the interaction of projectile atoms with targets under particle radiation in materials, e.g. in space applications or nuclear reactors, it is critical to investigate electronic and ionic contributions to stopping power. The goal of such efforts is detailed understanding of radiation damages as well as fundamental effects such as ion-electron interaction. While ionic stopping has been successfully modeled by molecular dynamics in the past, only recently a computational framework came within reach that is capable of accurately describing *electronic* stopping from first principles. Using our large-scale implementation of real-time time-dependent density functional theory in non-adiabatic Ehrenfest molecular dynamics, we are able to gain deep insight into electronic stopping for systems with hundreds of atoms and thousands of electrons, taking into account their quantum-mechanical electron-electron interaction. We discuss distinct contributions of valence and core electrons of aluminum target atoms to electronic stopping, and we study their importance for different projectile (hydrogen and helium atoms) velocities. There is striking influence of the stopping geometry especially for fast projectiles, and we find excellent agreement with experiment.

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