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Advances on Time-dependent DFT Simulations of Electronic Stopping[1] ALFREDO CORREA, ANDRE SCHLEIFE, Lawrence Livermore National Laboratory, YOSUKE KANAI, University of North Carolina at Chapel Hill, JORGE KOHANOFF, Queen's University, Belfast, ALFREDO J. CARO, Los Alamos National Laboratory — Radiation damage of reactor materials is a topic of interest and continuous research in the nuclear industry. A single nuclear decay event (e.g. alpha) produces a cascade of collisions involving the displacement of thousands of atoms in a crystalline material. While atomistic-scale simulations would be the ideal tool to understand these processes, the fact that they currently work on the assumption that electrons respond adiabatically to the atomic motion does not provide valid answers, for example to the stopping power problem. An alternative approach to attacking this problem is a method which explicitly takes into account electron non-adiabatic dynamics. We will present results obtained by time-depending DFT on the electronic stopping power of channeling protons in prototypical metals and insulators obtained by recent implementations of non-adiabatic electron dynamics methods.

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