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**Electronic stopping power from ab-initio Ehrenfest molecular dynamics** ANDRE SCHLEIFE, Lawrence Livermore National Laboratory, YOSUKE KANAI, The University of North Carolina at Chapel Hill, ALFREDO CORREA, Lawrence Livermore National Laboratory — Many materials are exposed to particle radiation: Metal walls of nuclear reactors in fission systems are subject to ion bombardment. Solar cells and semiconductor components in satellites are damaged by ions from cosmic rays. In order to achieve high radiation tolerance, it is essential to comprehend the interaction of fast projectiles with the ionic and electronic system of the target at a fundamental level. Based on the real-time propagation of time-dependent Kohn-Sham equations we developed a highly parallel plane-wave implementation of non-adiabatic Ehrenfest molecular dynamics, overcoming the adiabatic Born-Oppenheimer approximation. Thanks to the excellent scalability of our explicit integration scheme on supercomputers, it allows for the parameter-free computation of electronic stopping with hundreds of atoms in the calculation. We summarize our approach with some attention to important computational details. The influence of different charge states of H, He, and Li projectiles penetrating an Al target will be outlined. While we find good agreement with experiment up to the maximum of electronic stopping, deviations for high velocities are discussed in the light of the theoretical framework and off-channeling effects. Prepared by LLNL under Contract DE-AC52-07NA27344.

Andre Schleife
Lawrence Livermore National Laboratory

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