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Multiscale modeling of electron-ion dynamics in silicon under particle radiation ANDRE SCHLEIFE, CHENG-WEI LEE, Univ of Illinois - Urbana, KHALID HATTAR, REMI DINGREVILLE, STEPHEN FOILES, Sandia National Labs — Effects of fast ions impacting solids are important, in order to quantitatively understand radiation damage, ion beam modification (e.g. helium microscopy), or ion implantation. The interaction of a fast ion with kinetic energies in the MeV range and a target involves both electron-ion as well as ion-ion collisions. Ehrenfest molecular dynamics, based on real-time propagation of time-dependent Kohn-Sham equations, provides highly accurate insight into early stages of the defect-formation process and, in particular, into electronic stopping. Thanks to the excellent scalability of our plane-wave implementation, we are capable to perform these parameter-free simulations for supercells with hundreds of atoms using high-performance computing. However, the cost of Ehrenfest dynamics is prohibitively high for entire radiation-cascade development both regarding length- and time scales. Results from TDDFT for silicon targets are used to provide much more accurate information on velocity- and position-dependence of electronic stopping that we transfer into classical molecular dynamics. This results in a multi-scale simulation framework capable of studying crystalline semiconductors such as Si, GaP, or InP.

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