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Semiconductors Under Ion Radiation: Ultrafast Electron-Ion Dynamics in Perfect Crystals and the Effect of Defects CHENG-WEI LEE, ANDRÉ SCHLEIFE, University of Illinois at Urbana-Champaign — Stability and safety issues have been challenging difficulties for materials and devices under radiation such as solar panels in outer space. On the other hand, radiation can be utilized to modify materials and increase their performance via focused-ion beam patterning at nano-scale. In order to grasp the underlying processes, further understanding of the radiation-material and radiation-defect interactions is required and inevitably involves the electron-ion dynamics that was traditionally hard to capture. By applying Ehrenfest dynamics based on time-dependent density functional theory, we have been able to perform real-time simulation of electron-ion dynamics in MgO and InP/GaP. By simulating a high-energy proton penetrating the material, the energy gain of electronic system can be interpreted as electronic stopping power and the result is compared to existing data. We also study electronic stopping in the vicinity of defects: for both oxygen vacancy in MgO and interface of InP/GaP superlattice, electronic stopping shows strong dependence on the velocity of the proton. To study the energy transfer from electronic system to lattice, simulations of about 100 femto-seconds are performed and we analyze the difference between Ehrenfest and Born-Oppenheimer molecular dynamics.

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