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Electron-Ion Dynamics in Semiconductors with Defects under Ion Irradiation[1] CHENG-WEI LEE, ANDRÉ SCHLEIFE, University of Illinois at Urbana-Champaign — Long-term stability is challenging for semiconductor devices under ion radiation such as solar panels in outer space. Exposure to ion radiation induces formation of defects that ultimately reduce solar cell efficiency. It is well-known in the literature that high-energy ion radiation transfers energy to the materials mostly via electronic excitation which is traditionally hard to model. Previously, we demonstrated that Ehrenfest molecular dynamics based on time-dependent density functional theory correctly describes electronic stopping of semiconductors. To better understand the effect of excited electrons on evolution of defects during ion irradiation, we further investigate the time-evolution of occupation number and found that it is correlated to long-term ion dynamics after passage of proton. Furthermore, we found that the presence of excited electrons significantly reduces the atomic diffusion barrier, indicating this effect is essential for the analysis of defect formation and ion dynamics under ion radiation conditions.

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