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Title: Charge Transfer and Redistribution during Low-Energy Recoil Events

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Silicon carbide is a material of great interest for fission and fusion energy systems, and Y-Ti-O systems are of interest as nanoscale precipitates that enhance radiation resistance in ODS alloys for structural applications in fission reactors. We have used ab initio molecular dynamics methods to study the electronic charge transfer and redistribution that occurs during defect production from low-energy recoil events in SiC and Y2Ti2O7. In addition, density functional theory methods have been used to investigate the relative stability and electronic structure of the resulting defect configurations. In SiC, significant charge-transfer occurs during the recoil event, and the charge variation of the recoil atom can decrease the energy barrier for stable defect formation, leading in some cases to a charged defect. In the case of Y2Ti2O7, low-energy cation recoils are found to prefer coming to rest in vacant 8a anion sites and in bridge sites between two neighboring cations along the direction, rather than the cation-cation dumbbell interstitial configurations predicted by classical molecular dynamics. Density functional theory calculations reveal that these unexpected cation interstitial configurations are very stable and exhibit metallic-like bonding with nearest neighbor cations, and density of state analysis demonstrates that some electrons distribute around the Fermi level, indicating a local metallic ground state.