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Real-Time Time-Dependent DFT Study of Electronic Stopping in Semiconductors under Proton Irradiation DILLON C. YOST, KYLE G. REEVES, YOSUKE KANAI, University of North Carolina - Chapel Hill — Understanding the detailed mechanisms of how highly energetic charged particles transfer their kinetic energy to electronic excitations in materials has become an important topic in various technologies ranging from nuclear energy applications to integrated circuits for space missions. In this work, we use our new large-scale real-time time-dependent density functional theory simulation [1] to investigate details of the ion-velocity-dependent dynamics of electronic excitations in the electronic stopping process. In particular, we will discuss how point defects in semiconductor materials influence the electronic stopping process under proton irradiation, using silicon carbide (3C-SiC) as a representative material due to its great technological importance. Additionally, we will provide atomistic insights into existing analytical models that are based on the plane-wave Born approximation by examining velocity-dependence of the projectile charge from first-principles simulations. [1] "Quantum Dynamics Simulation of Electrons in Materials on High-Performance Computers" A. Schleife, E. W. Draeger, V. Anisimov, A. A. Correa, Y. Kanai, Computing in Science and Engineering, 16 (5), 54 (2014).

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