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First-Principles Investigation of Electronic Excitation Dynamics in Water under Proton Irradiation KYLE REEVES, YOSUKE KANAI, Univ of NC - Chapel Hill — A predictive and quantitative understanding of electronic excitation dynamics in water under proton irradiation is of great importance in many technological areas ranging from utilizing proton beam therapy to preventing nuclear reactor damages. Despite its importance, an atomistic description of the excitation mechanism has yet to be fully understood. Identifying how a high-energy proton dissipates its kinetic energy into the electronic excitation is crucial for predicting atomistic damages, later resulting in the formation of different chemical species. In this work, we use our new, large-scale first-principles Ehrenfest dynamics method [1,2] based on real-time time-dependent density functional theory to simulate the electronic response of bulk water to a fast-moving proton. In particular, we will discuss the topological nature of the electronic excitation as a function of the proton velocity. We will employ maximally-localized functions to bridge our quantitative findings from first-principles simulations to a conceptual understanding in the field of water radiolysis. [1] "Plane-wave Pseudopotential Implementation of Explicit Integrators for Time-Dependent Kohn-Sham Equations in Large Scale Simulations" A. Schleife, E. W. Draeger, Y. Kanai, A. A. Correa, J. Chem. Phys., 137, 22A546 (2012) [2] "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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