Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Electronic stopping in liquid water from first principles: An application of large-scale real-time TDDFT simulations KYLE REEVES, YI YAO, YOSUKE KANAI, University of North Carolina at Chapel Hill — Electronic stopping describes the transfer of energy from a highly-energetic charged particle to electrons in a material. This process induces massive electronic excitations via interaction between the material and the highly localized electric field from the charged particle. Understanding this phenomenon in condensed matter systems under proton irradiation has implications in various modern technologies. First-principles simulations, based on our recently-developed large-scale real-time time-dependent density functional theory approach, provide a detailed description of how electrons are excited via a non-equilibrium energy transfer from protons on the attosecond time scale. We apply this computational approach to the important case of liquid water under proton irradiation. Our work reveals several key features of the excitation dynamics at the mesoscopic and molecular levels which support a clearer understanding of the water radiolysis mechanism under proton irradiation. Importantly, we will demonstrate a first-principles determination of the energy transfer rate, (i.e. electronic stopping power) in liquid water, and a comparison to existing empirical models will be presented. We will conclude by discussing how the exchange-correlation approximation influences the calculation of the electronic stopping power.

Kyle Reeves
University of North Carolina at Chapel Hill

Date submitted: 06 Nov 2015 Electronic form version 1.4