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Examining Physical and Numerical Approximations in Real-Time TDDFT Non-Equilibrium Dynamics Simulations for Determining Electronic Stopping Power DILLON C. YOST, University of North Carolina - Chapel Hill, YI YAO, University of North Carolina at Chapel Hill, YOSUKE KANAI, University of North Carolina - Chapel Hill — The accurate prediction of electronic stopping power, the rate of energy transfer from swift ions to electrons in matter, is of great importance in developing future technologies in areas such as nuclear energy, space electronics, and thermal neutron detection. In recent years, real-time time-dependent density functional theory (RT-TDDFT) has been employed to calculate electronic stopping power from first principles. While the predictions from these first-principles non-equilibrium simulations agree very well with experimental data for ion velocities below the so-called Bragg peak of the electronic stopping power curve, in all cases there remains a significant underestimation of experimental results beyond the Bragg peak. In this work, we thoroughly inspect the details of RT-TDDFT electronic stopping simulations by examining various physical and numerical approximations employed in practical calculations.

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