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Non-adiabatic electron-ion dynamics in proton irradiated aluminum sheets ALINA KONONOV, ANDRE SCHLEIFE, University of Illinois at Urbana-Champaign — Ion-irradiation of materials enables techniques like ion beam microscopy and can lead to material degradation in space and nuclear technology. Thin or two-dimensional materials respond to ion-irradiation differently than their bulk counterparts, and characterizing this pre-equilibrium response is essential for developing applications. We use Ehrenfest dynamics to simulate a 25 keV proton traversing a $0.8-1.6$ nm thick aluminum sheet at a proton dose of 2.4×10^{13} cm^{-2}. We analyze the time-dependent electron density to obtain the entrance-side and exit-side secondary electron yields and the orbital occupations of the exiting projectile. From our results for position-dependent stopping in the target, we also compute the effective charge of the projectile inside the target. Finally, we consider the dependence of these quantities on target thickness. Our approach overcomes challenges posed by artificial interaction between entrance-side and exit-side secondary electron densities and integration error accumulated after propagating Kohn-Sham orbitals for thousands of time steps in large simulation volumes.

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