

Abstract Submitted
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Ultrafast Electron-Ion Dynamics Near Aluminum Surfaces ANDRE SCHLEIFE, KAI WELLS, SAM KNEWSTUB, Univ of Illinois - Urbana — Computational physics and materials research have greatly benefited from high-performance computing; modern first-principles simulations allow insight with unprecedented accuracy and detail. Here we use a recent highly parallel implementation of Ehrenfest molecular dynamics based on real-time time-dependent density functional theory to describe non-adiabatic ultrafast electron-ion dynamics using accurate first-principles calculations. We investigate aluminum subject to highly energetic particle radiation (hydrogen projectile) and study energy deposition due to the fast projectiles. Their high velocity makes it necessary to overcome the Born-Oppenheimer approximation. Using our first-principles calculations we study the behavior of fast ions near the surface of aluminum slabs and investigate, for instance, the influence of velocity and impact angle of the projectile ion. From the emerging non-adiabatic electron-ion dynamics we gain insight into the material on an atto-second time scale.

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