Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Massively Parallel Real-Time TDDFT Simulations of Electronic Stopping Processes DILLON YOST, University of North Carolina at Chapel Hill, CHENG-WEI LEE, University of Illinois at Urbana-Champaign, ERIK DRAEGER, ALFREDO CORREA, Lawrence Livermore National Laboratory, ANDRE SCHLEIFE, University of Illinois at Urbana-Champaign, YOSUKE KANAI, University of North Carolina at Chapel Hill — Electronic stopping describes transfer of kinetic energy from fast-moving charged particles to electrons, producing massive electronic excitations in condensed matter. Understanding this phenomenon for ion irradiation has implications in modern technologies, ranging from nuclear reactors, to semiconductor devices for aerospace missions, to proton-based cancer therapy. Recent advances in high-performance computing allow us to achieve an accurate parameter-free description of these phenomena through numerical simulations. Here we discuss results from our recently-developed large-scale real-time TDDFT implementation for electronic stopping processes in important example materials such as metals, semiconductors, liquid water, and DNA. We will illustrate important insight into the physics underlying electronic stopping and we discuss current limitations of our approach both regarding physical and numerical approximations. This work is supported by the DOE through the INCITE awards and by the NSF. Part of this work was performed under the auspices of U.S. DOE by LLNL under Contract DE-AC52-07NA27344.

Yosuke Kanai
University of North Carolina at Chapel Hill

Date submitted: 11 Nov 2016 Electronic form version 1.4