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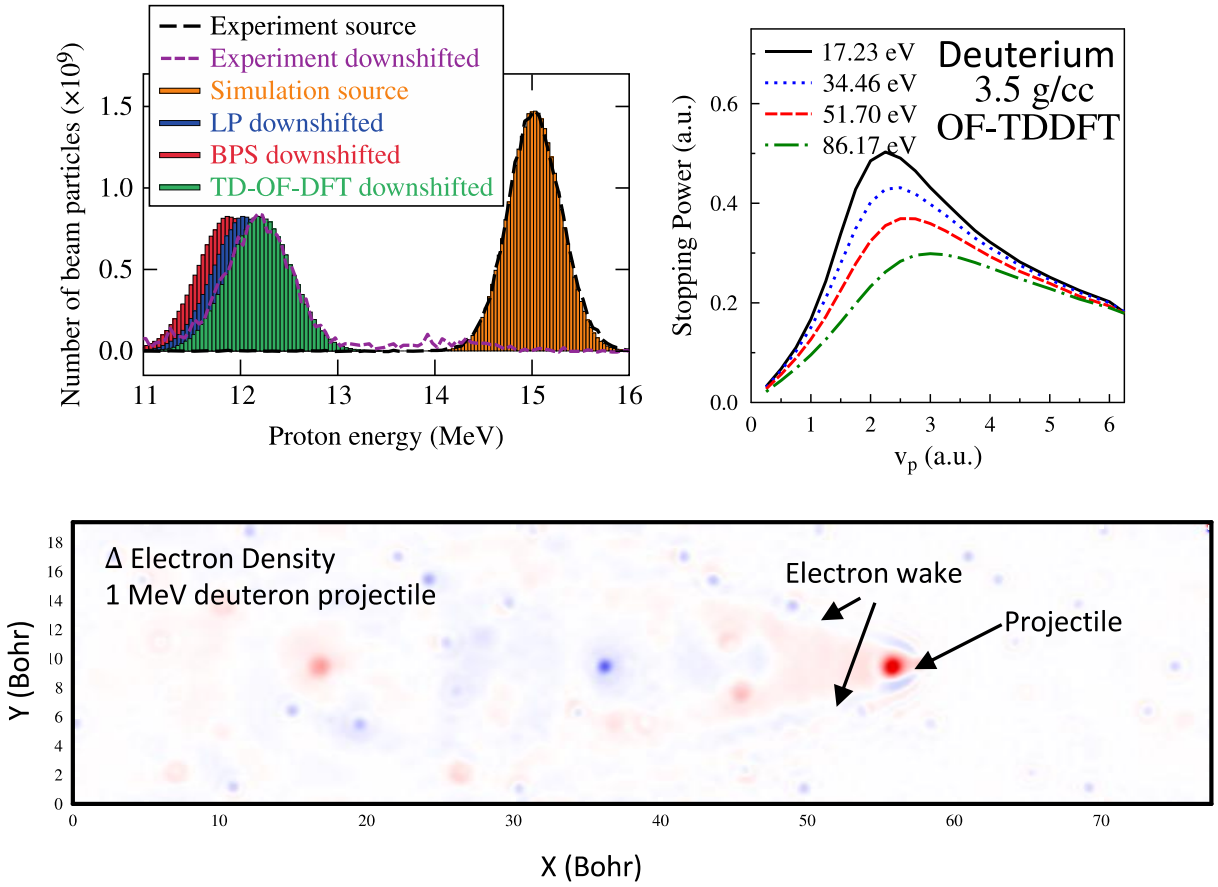
Ab-Initio Stopping power in the warm dense matter regime by Orbital-Free Time Dependent DFT

A novel orbital-free density functional theory approach provides *ab-initio* simulations of nonadiabatic stopping power in the previously inaccessible hot and warm dense matter environment.



Left-Top: Experimental & simulated alpha particle projectile velocity distributions before & after stopping by warm dense Beryllium ($k_BT = 32\ eV$, $\rho = 1.78\ g/cc$). Right-Top: TD-OF-DFT calculated deuteron stopping power of warm & hot dense Deuterium ($\rho = 3.5\ g/cc$), up to 1 million Kelvin. Bottom: TD-OF-DFT simulated electron density difference, showing the full simulation window (1029 atoms).

The Science

A collaboration between researchers at the Laboratory for Lase Energetics at the University of Rochester (LLE), and the Computer, Computational and Statistical Science and Theoretical Divisions at Los Alamos National Laboratory (LANL) has developed a novel approach to the simulation of *first-principles* nonadiabatic stopping power. Based on a time-dependent orbital-free density functional theory (TD-OF-DFT), this new approach allows numerically tractable simulations of, experimentally relevant, high electronic temperature and density plasmas. Large simulation cells, required to overcome finite-size effects, and high temperatures have prohibited orbital-based TD-DFT simulations in this regime. A new non-adiabatic kinetic energy density functional, which depends on the local current density, is introduced to accurately capture the electron response to low and near-peak energy projectiles in the orbital-free framework. Using this new technique, simulations of stopping power of alpha-particles by warm dense beryllium are in excellent agreement with recent experimental measurement as compared to analytical models. The orbital-free TDDFT approach is also compared to orbital-based TD-DFT for stopping of deuterons by warm-dense Deuterium.

The Impact

Stopping power is a key quantity in modeling internal confinement fusion (ICF) and other high energy density (HEDP) process where fusion products are slowed by background plasma. The development of *ab initio* methods that can simulate electronic response in warm and hot dense plasmas is critical to the advancement of modeling capabilities in multiple areas including ICF, weapons physics, planetary and stellar systems, etc. The proposed time-dependent orbital-free density functional theory approach could significantly extend the parameter range which can be accurately simulated using *first-principles*.

Summary

Stopping of swift ions by electrons is a critical process in high energy density physics, including internal confinement fusion, weapons physics, and planetary or stellar science. Stopping power simulations of systems at high temperatures and high densities, *i.e.* warm or hot dense matter, pose a particular challenge, due to numerical and theoretical complications and the large system sizes required. This new method is numerically tractable for such high temperature, high density, systems and is in excellent agreement with available experimental data. The path may open the way for simulation of other electronic response properties such as electrical and thermal conductivities and opacities in previously inaccessible warm and hot dense matter environments.

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Publications

Y. H. Ding, A. J. White, S. X. Hu, O. Certik, L. A. Collins, "Ab Initio Studies on the Stopping Power of Warm Dense Matter with Time-Dependent Orbital-Free Density Functional Theory" *Physical Review Letters* **121**, 145001 (2018)

A. J. White, O. Certik, Y. H. Ding, S. X. Hu, L. A. Collins, "Time-dependent orbital-free density functional theory for electronic stopping power: Comparison to the Mermin-Kohn-Sham theory at high temperatures" *Physical Review B* **98**, 144302 (2018)

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