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Nonadiabatic Ab-initio Simulations: Ab Initio Stopping Power of High Energy Ions[1]

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We perform ab initio simulations of electronic, ionic, and nonadiabatic dynamics in the warm dense matter (WDM) and hot dense plasma (HDP) regimes. Using density-functional theory (DFT) in two guises: orbital-based Kohn-Sham (KS) and orbital-free (OF) Thomas-Fermi-Dirac approximations, permits a wide coverage of extreme conditions. This approach provides a consistent set static, dynamic, and optical properties such as equation of state, mass transport, opacity, conductivity and ion stopping power. We have developed explicitly time-dependent (TD) versions of both the KS and OF approaches in order to treat electron conductivities and stopping power. The TD schemes offer a path into the upper ranges of the WDM regime, into HDP. Additionally, the response to high frequency (temporal) perturbations can be simulated, as can non-linear or non-equilibrium interactions, *e.g.* between the plasma and an intense laser pulse. Our recent simulations of the, inherently non-linear and non-adiabatic, electronic stopping of high energy ions will be presented. The efficiency of OF TD-DFT allows for large simulation sizes at high temperatures. This is required for the direct calculation of stopping power for MeV projectiles, relevant to ICF plasma heating. Comparison of OF and KS stopping show excellent agreement for high velocities. We have derived a current-dependent kinetic energy functional that improves agreement at low velocities.

1. Y.H. Ding, A.J.White, O. Certik, S.X. Hu, and L.A. Collins, "Ab initio studies of stopping power in warm dense matter using time-dependent density functional theory," *Phys. Rev. Lett.* **121**, 145001

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

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