First-principles benchmarks for electronic response of warm dense matter

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Hydrodynamic simulations used to design and interpret fusion experiments rely on tabulated material properties over a wide range of pressures and temperatures as the target evolves from ambient conditions to a burning plasma. The intermediate warm dense regime presents unique challenges because models struggle to capture coexisting thermal and quantum effects accurately, while experimental characterization is rare and often suffers from large uncertainties. Here, we review ongoing work to advance computational methods for predicting electronic response properties of warm dense matter, including stopping power, x-ray scattering spectra, and conductivity. Using real-time time-dependent density functional theory (TDDFT), we benchmark and constrain efficient treatments based on average-atom methods and model dielectric functions [1-3]. Since the reliability of these more approximate models then depends on the credibility of the first-principles data, we scrutinize the methodological choices of the TDDFT calculations and show that sensitivities to pseudopotential details, projectile trajectory, and finite-size effects can lead to significant errors in computed stopping powers of around 15% [4,5]. We also discuss collective, nonlinear, and subtle band structure effects that are predicted by TDDFT, carry important implications for accurately simulating and diagnosing warm dense matter, and remain difficult for simplified models to capture [3]. Finally, we consider the prospects of emerging quantum computing technologies enabling even more precise benchmark calculations [6].

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