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Improving warm dense matter models with accurate first-principles benchmarks

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Quantum degeneracy and thermal effects challenge atomic models of warm dense matter (WDM), a regime where partial ionization, interatomic bonding, and band structure can modify plasma response properties. We use real-time time-dependent density functional theory (TDDFT), a multi-center first-principles approach, to benchmark the predictions of an improved average-atom (AA) framework for WDM. Our comparisons of dynamic structure factors in warm dense deuterium, carbon, and aluminum help constrain models of electron-ion collision frequencies that broaden and shift the plasmon feature often analyzed in x-ray scattering diagnostics. However, TDDFT also predicts other effects that remain difficult for AA to capture. First, we find that collective behavior in warm dense iron blue shifts transitions into thermally depleted d states. Also, we uncover subtle signatures of atomic order in isochorically heated aluminum arising from non-idealities in the density of states. But despite its higher accuracy relative to AA, TDDFT still relies on some poorly characterized and difficult to improve approximations. We will conclude with a preview of some potential advantages that emerging quantum computing technologies may offer for modeling atomic processes in plasmas. This work has important implications for WDM modeling and characterization, most immediately the possibility of novel diagnostic techniques for high temperatures and/or systems out of thermal equilibrium.

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