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Warm Dense Matter Demonstrating Non-Drude Conductivity from Observations of Nonlinear Plasmon Damping[1]

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The thermal and electrical conductivity, equation of state and the spectral opacity in warm dense matter (WDM) are essential properties for modeling, e.g., fusion experiments or the magnetic field generation in planets. In the last decade it has been shown that x-ray Thomson scattering (XRTS) is an effective tool to determine plasma parameters like temperature and density in the WDM regime[2]. Recently, the electrical conductivity was extracted from XRTS experiments for the first time[3]. The spectrally resolved scattering data of aluminum, isochorically heated by the Linac Coherent Light Source (LCLS), show strong dependence on electron correlations. Therefore, the damping of plasmons, the collective electron oscillations, has to be treated beyond perturbation theory.
We present results for the dynamic transport properties in warm dense aluminum using density-functional-theory molecular dynamics (DFT-MD) simulations. The choice of the exchange-correlation (XC) functional, describing the interactions in the electronic subsystem, has significant impact on the ionization energy of bound electrons and the dynamic dielectric function. Our newly developed method for the calculation of XRTS signals including plasmon and bound-free transitions is based on transition matrix elements together with ionic contributions using uniquely DFT-MD simulations. The results show excellent agreement with the LCLS data if hybrid functionals are applied[4]. The experimental finding of nonlinear plasmon damping is caused by the non-Drude conductivity in warm dense aluminum. Here, we show further validation by comparing with x-ray absorption data. These findings enable new insights into the impact of XC functionals on calculated properties of WDM and allow detailed predictions for future experiments at the unprecedented densities on the NIF.

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