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First-principles calculations of dynamic transport properties for x-ray Thomson scattering experiments on warm dense aluminum BASTIAN B. L. WITTE, University of Rostock, SLAC National Accelerator Laboratory, PHILIPP SPERLING, European XFEL, SLAC National Accelerator Laboratory, SIEGFRIED H. GLENZER, SLAC National Accelerator Laboratory, RONALD REDMER, University of Rostock — X-ray Thomson scattering (XRTS) is an effective tool to determine plasma parameters, e.g., temperature and density, in the warm dense (WD) matter regime. Furthermore, transport coefficients are relevant for modeling, e.g., fusion experiments or the magnetic field generation in planets. Recently, the electrical conductivity was extracted for the first time from XRTS experiments on aluminum, isochorically heated by the Linac Coherent Light Source (LCLS) [1]. The measured spectrally resolved scattering signal shows a strong dependence on the electron interactions, which have to be treated beyond perturbation theory. We present results for the dynamic transport properties in WD 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 potential and the thermal and electrical conductivity. The calculation of the XRTS signal from the DFT-MD simulations shows very good agreement with the LCLS data [1] if hybrid functionals are applied, i.e., XC functionals within the generalized gradient approximation are not suitable for the description of WD aluminum. [1] P. Sperling et al., Phys. Rev. Lett. 115, 115001 (2015)

Bastian Bernhard Lothar Witte
University of Rostock, SLAC National Accelerator Laboratory

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