Abstract Submitted
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**Influence of exchange-correlation temperature effects on electric conductivity of aluminum in WDM regime**[1] VALENTIN KARASIEV, LÁZARO CALDERíN, SAM TRICKEY, Physics Dept., Univ. Florida — Calculation of transport properties in the warm dense matter (WDM) regime and comparison with experiment is an important development challenge. Computationally affordable, reliable theoretical methods are required. Current best practice is Kohn-Sham molecular dynamics (KS-MD) to sample ionic configurations and Kubo-Greenwood (KG) conductivity calculations at selected configurations. Relevant aspects are (i) the very high computational cost and unfavorable cost-scaling of the KS-MD at WDM temperatures, and (ii) neglect of explicit temperature effects in the ground state exchange-correlation (XC) functionals often used to approximate the XC free energy. We address both issues. We sample configurations of aluminum ions in the WDM regime with drastically lowered MD cost via finite-temperature orbital-free MD, including explicitly T-dependent XC [1]. Then we delineate the XC T-effects by comparing KG conductivities calculated with and without explicit XC T-dependence. The result is that explicitly T-dependent XC gives an unequivocal improvement with respect to experiment for aluminum at low material density and elevated temperatures. [1] V.V. Karasiev, T. Sjostrom, J. Dufty, and S.B. Trickey, Phys. Rev. Lett. 112, 076403 (2014)

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