Abstract Submitted
for the DPP20 Meeting of
The American Physical Society

Finite temperature density functional theory investigation of the electrical conductivity of warm dense matter with peculiar electronic structure within a two-temperature model SHEN ZHANG, Kiel University, National University of Defense Technology, HENGYU ZHANG, JIAYU DAI, National University of Defense Technology, MICHAEL BONITZ, Kiel University — Density functional theory (DFT) is widely used to investigate the properties of warm dense matter (WDM), including the equation of state, structural properties, as well as transport properties such as thermal and electrical conductivity. However, the common usage of ground state exchange correlation functionals undermines the reliability of DFT calculations since the electron temperature in the WDM regime is far beyond zero. Applying the Kubo-Greenwood formula, we present a DFT investigation of the electrical conductivity of warm dense lithium, aluminum, copper and gold with peculiar electronic structure that has electron holes for a two-temperature situation, which can be realized in the lab by isochoric heating techniques. Comparing the novel finite-temperature exchange correlation functional (FTXC) of Ref. [1] with the widely used ground state expressions, we reexamine the temperature effect of electrons in WDM[2]. This work is helpful to better understand the physics of related WDM experiments.

[1]S. Groth *et al.*, Phys. Rev. Lett. **119**, 135001 (2017)
[2]M. Bonitz *et al.*, Phys. Plasmas **27**, 042710 (2020)

Shen Zhang
Kiel University, National University of Defense Technology

Date submitted: 28 Jun 2020 Electronic form version 1.4