Contribution ID: **28** Type: **not specified**

Thermal PBE for Warm Dense Matter Calculations

Friday 16 September 2022 11:00 (30 minutes)

Finite-Temperature Density Functional Theory (FT-DFT) has played a significant role in the study of warm dense matter over the past few decades. However, modern FT-DFT calculations typically make use of ground-state approximations to the exchange-correlation (XC) free energy, ignoring its temperature dependence. While overall the ground-state approximation is valid in both the low- and high-temperature limits, the quantitative ramifications of this approximation are unknown and may be crucial to our current understanding of warm dense matter. To correct this, we calculate the temperature dependence of PBE through a sequence of Kohn-Sham CP-DFT calculations [1] that yield accurate exchange-correlation holes at finite temperatures. We will present the results of this thermal PBE and compare with existing suggestions in the literature.

[1] R. J. McCarty, et al. "Bypassing the Energy Functional in Density Functional Theory: Direct Calculation of Electronic Energies from Conditional Probability Densities."Phys. Rev. Lett. 125, 266401 (2020).

We acknowledge funding from the Department of Energy Award No. DE-FG02-08ER46496.

Primary author: KOZLOWSKI, John (University of California, Irvine, United States)

Co-author: BURKE, Kieron

Presenter: KOZLOWSKI, John (University of California, Irvine, United States)

Session Classification: Morning Session (Friday)