Abstract Submitted
for the FWS15 Meeting of
The American Physical Society

Thermal Corrections to Density Functional Simulations of Warm Dense Matter JUSTIN SMITH, AURORA PRIBRAM-JONES, KIERON BURKE, University of California, Irvine — Present density functional calculations of warm dense matter often use the Mermin-Kohn-Sham (MKS) scheme at finite temperature, but employ ground-state approximations to the exchange-correlation (XC) free energy. In the simplest solvable non-trivial model, an asymmetric Hubbard dimer, we calculate the exact many-body energies, the exact Mermin-Kohn-Sham functionals for this system, and extract the exact XC free energy. For moderate temperatures and weak correlation, we show this approximation is excellent, but fails for stronger correlations. Additionally, we use this system to test various conditions that must be satisfied.

Justin Smith
University of California, Irvine

Date submitted: 12 Oct 2015 Electronic form version 1.4