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Finite-Temperature Orbital-free Density Functional Calculations for Warm Dense Lithium[1] V.V. KARASIEV, T. SJOSTROM, S.B. TRICKEY, Univ. of Florida, Physics, QTP — Warm dense matter (WDM) defines the region between condensed matter and plasmas. This regime is characterized by high pressure and elevated temperature. The standard theoretical and computational approach, which is a combination of finite-temperature Kohn-Sham density functional theory (KS-DFT) and classical molecular dynamics, becomes computationally very expensive at elevated temperature. The orbital-free (OF) version of DFT is a less expensive alternative to the orbital-based methods. We have implemented finite-temperature Thomas-Fermi, second-order gradient expansion, and new generalized gradient approximation free energy functionals in an OF-DFT code. These non-interacting free-energy functionals are used in combination with zero-temperature exchange-correlation in local density approximation. Self-consistent OF-DFT calculations with these functionals are performed for lithium for the range of densities $\rho_{\mathrm{Li}} = 0.5 - 10$ g/cm^3 and temperatures between 100 K and 100 kK. OF-DFT results are compared to the standard Kohn-Sham data. Local pseudopotentials used on OFDFT calculations are validated by comparison between Kohn-Sham results obtained with standard non-local pseudopotentials and with the same local pseudopotentials.

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