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Density Functional versus Thermal Hartree-Fock Approximations in Warm Dense Lithium[1] VALENTIN V. KARASIEV, TRAVIS SJOSTROM, S.B. TRICKEY, Quantum Theory Project, Physics Dept. U. Florida — We compare the behaviors of the thermal Hartree-Fock (tHF) model and thermal Density Functional Theory (tDFT) using both ground-state and temperature-dependent approximate functionals. The test system is bcc Li in the temperature-density regime of warm dense matter. In the exchange-only case, we find significant qualitative differences between the exact tHF and the DFT calculations with zero-temperature local density approximation (LDA) exchange. A temperature-dependent LDA functional provides much better agreement with the tHF exchange. An underlying need is for well-characterized, reliable pseudopotentials over demanding temperature and density ranges. Thus we compare pseudopotential and all-electron results for small Li clusters of local bcc symmetry and bond-lengths appropriate to high density bulk Li. We determine the density range over which both standard projector-augmented wave(PAW) and norm-conserving pseudopotentials are reliable. Then we construct small-cutoff-radius PAW data sets (for both the local density and the generalized gradient exchange-correlation approximations) which are valid for lithium densities up to at least 80 g/cm^3.

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