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Finite-temperature Exchange and Correlation Functionals in Self-Consistent Calculations[1] T. SJOSTROM, V.V. KARASIEV, S.B. TRICKEY, University of Florida — Density functional theory is being used increasingly to investigate systems at substantial electron temperatures (e.g., warm dense matter, order of 1-10 eV or more). A common approach uses a ground-state (zero-temperature) exchange-correlation (XC) functional with thermal occupancy (Fermi distribution) of the Kohn-Sham states. Various finite-temperature extensions for XC free energy (Sommerfeld expansion, RPA, STLS, classical map) have been proposed, however. All have LDA form. We have implemented several in a pseudopotential code (SIESTA), and also extended them to have the PBE-GGA as the zero-temperature limit. We report equation of state calculations for Li from ambient density and temperature through the warm dense matter regime. Nontrivial variation is found.

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