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Construction of Generalized Gradient Approximation Free Energy Density Functionals[1] SAM TRICKEY, VALENTIN KARASIEV, TRAVIS SJOSTROM, QTP, Physics and Chemistry, U. Florida — By analyis of the second-order gradient approximation (SGA) for the non-interacting electron free energy density, we propose a finite-temperature generalized gradient approximation (ftGGA) for the noninteracting free energy density (both kinetic and entropic contributions). By analogy we also introduce a ftGGA for the exchange free energy density functional. We have implemented the finite-temperature Thomas-Fermi (ftTF), SGA, and a new finite-temperature GGA free-energy functional in the orbital-free density functional theory (OFDFT) code PROFESS. We compare self-consistent OFDFT results with standard Kohn-Sham data. The local pseudopotentials used in the 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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