Structure of Generalized Gradient Approximation Free Energy Density Functionals

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Development of approximate functionals for finite-temperature density functional theory (ftDFT) calculations lags substantially compared to the refinement achieved for ground-state functionals. To develop the structure of finite-temperature generalized gradient approximations (ftGGA) for the kinetic and entropic contributions to the non-interacting free energy, we analyze the second-order gradient approximation (SGA). We also introduce the analogous ftGGA for the exchange free energy density functional. We have implemented the finite-temperature Thomas-Fermi (ftTF) and SGA functionals, as well as 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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