Developing a Laplacian-Level Framework for Noninteracting Free-Energy Density Functionals

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A framework is developed for orbital-free Laplacian-level meta-generalized-gradient-approximation (meta-GGA) for the noninteracting free energy and its components (kinetic energy, entropic term) density functionals based upon analysis of the fourth-order gradient expansion. A nonempirical functional that correctly reproduces the finite-temperature fourth-order gradient expansion for the noninteracting free energy is constructed. Preliminary meta-GGA results for warm dense helium show that the reliable applicability of orbital-free density functional theory-based molecular-dynamics simulations has been pushed down to the low-temperature range of ~7 eV from ~30 to 40 eV at the GGA level of theory [1–3].

1. V. V. Karasiev, T. Sjostrom, and S. B. Trickey, Phys. Rev. B **86**, 115101 (2012).
2. V. V. Karasiev, D. Chakraborty, O. A. Shukruto, and S. B. Trickey, Phys. Rev. B **88**, 161108(R) (2013).
3. K. Luo, V. V. Karasiev, and S. B. Trickey, Phys. Rev. B **101**, 075116 (2020).