Meta-GGA Exchange-Correlation Free-Energy Density Functional: Achieving Unprecedented Accuracy for Warm-Dense-Matter Simulations

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Accurate knowledge of equation of state, transport and optical properties describing possible phase transitions across the warm-dense-matter (WDM) regime plays an important role in planetary science, astrophysics, and inertial confinement fusion. *Ab initio* molecular dynamics (AIMD) simulations based on *free-energy* density functional theory (DFT), in combination with the Kubo–Greenwood (KG) formulation for transport and optical properties, has proven to be a successful and key tool to understanding WDM and high-energy-density plasmas across different temperature regimes. DFT requires approximations for the exchange-correlation (XC) energy density functional. A common approximation is to use a ground-state XC functional, which does not consider any explicit XC thermal effects.

We present strategies for thermalization of the ground-state meta-generalized gradient approximation (meta-GGA) XC functionals to treat XC thermal effects explicitly. A simple but accurate scheme is implemented via universal additive thermal correction to XC using a perturbative-like self-consistent approach. The additive correction with explicit temperature dependence is applied to the ground-state deorbitalized, strongly constrained and appropriately normed (SCAN-L) meta-GGA XC, leading to thermal XC functional denoted as T-SCAN-L. The thermal T-SCAN-L meta-GGA functional shows significant improvement in DFT calculation accuracy for warm dense matter by a factor of 3 to 10, achieving unprecedented accuracy of total pressure between a few tenths and ~1% when compared to thermal GGA and traditional ground-state XC functionals, as demonstrated by the comparison to path-integral Monte Carlo simulations for helium and hydrogen equation of state.

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