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The importance of the finite-temperature exchange-correlation for warm dense matter studies[1] V.V. KARASIEV, S.B. TRICKEY, Physics and QTP, Univ. Florida — Matter at extremely elevated temperature (thousands to millions Kelvin) under a wide range of pressures usually is treated by ab initio molecular dynamics driven by free-energy DFT. Whether in the Kohn-Sham or orbital-free forms, implementation requires a reliable exchange-correlation (XC) free energy approximation. Finite-temperature Hartree-Fock calculations [1] suggest strongly that the explicit T-dependence of X is important. The recently developed first rung XC free-energy functional, the finite-T local density approximation (LDA) [2], captures that explicit T-dependence for the homogeneous electron gas. We report study of the impact of explicit T-dependence in the LDA on the properties of matter in the warm dense regime and conclude that there is a need to develop a T-dependent and density gradient-dependent XC functional. Next, we analyze the finite-T gradient expansion for X and C, extract from it the appropriate reduced density gradients for X and C with explicit T-dependence, introduce the next-rung GGA XC free-energy functionals, and discuss their behavior and properties.

[1] V.V. Karasiev, T. Sjostrom, and S.B. Trickey, Phys. Rev. E 86, 056704 (2012).
[2] V.V. Karasiev, T. Sjostrom, J. Dufty, and S.B. Trickey, Phys. Rev. Lett. 112, 076403 (2014).

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