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Development of Fast and Reliable Free-Energy Density Functional Methods for Simulations of Dense Plasmas from Cold- to Hot-Temperature Regimes V.V. KARASIEV, Laboratory for Laser Energetics, U. of Rochester — Free-energy density functional theory (DFT) is one of the standard tools in high-energy-density physics used to determine the fundamental properties of dense plasmas, especially in cold and warm regimes when quantum effects are essential. DFT is usually implemented via the orbital-dependent Kohn–Sham (KS) procedure. There are two challenges of conventional implementation: (1) KS computational cost becomes prohibitively expensive at high temperatures; and (2) ground-state exchange-correlation (XC) functionals do not take into account the XC thermal effects.[1] This talk will address both challenges and report details of the formal development of new generalized gradient approximation (GGA) XC free-energy functional which bridges low-temperature (ground state) and high-temperature (plasma) limits.[2] Recent progress on development of functionals for orbital-free DFT as a way to address the second challenge will also be discussed. This material is based upon work supported by the Department of Energy National Nuclear Security Administration under Award Number DE-NA0001944.

[1]V.V. Karasiev, L. Calderin, and S.B. Trickey, Phys. Rev. E **93**, 063207 (2016).
[2]V.V. Karasiev, J.W. Dufty, and S.B. Trickey, "Non-Empirical Semi-Local Free-Energy Density Functional for Matter Under Extreme Conditions," submitted to Physical Review Letters.

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