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Progress in Development of Thermal Hybrid Exchange-Correlation Density Functionals for Improving the Description of Warm Dense Matter[1] DEYAN MIHAYLOV, VALENTIN KARASIEV, SUXING HU, Laboratory for Laser Energetics, University of Rochester — Recently, it has been shown that explicit dependence on temperature T in the exchange-correlation (XC) free-energy density functional is important in density functional theory studies of warm dense matter. As a first approximation, the finite-T, non-empirical KSDT local spin-density approximation (LSDA) functional was constructed by analytical parametrization of the XC free energy of the homogeneous electron gas. Consequently, the KDT16 generalized gradient approximation (GGA) functional, which captures non-homogeneity effects and shows better agreement with experiments, was constructed. Here, we present progress in climbing the (finite-T) Jacob's ladder of XC functional approximations beyond the GGA, by developing a finite-T extension of the well-established PBE0 and HSE06 hybrids. Application to static calculations of electronic band gap at a wide range of T for various systems of interest to high-energy-density physics show that thermal hybrids provide a significant improvement to the LSDA and GGA rung XC functionals and to the ground-state PBE0 and HSE06 hybrids.

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