Abstract Submitted
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Finite-temperature orbital-free GGA molecular dynamics for warm dense hydrogen[1] VALENTIN KARASIEV, T. SJOSTROM, S.B. TRICKEY, Physics and QTP, Univ. Florida — The computational description of warm dense matter (WDM) by means of a combination of the Kohn-Sham (KS) finite-temperature density functional theory (DFT) for the electrons and classical molecular dynamics (MD) for the ions becomes an intractable task at high T (typically a few hundred kK). Finite-temperature orbital free DFT (OF-DFT) is a less expensive alternative. Only two non-interacting free-energy functionals for OF-DFT had been published and used until recently: the finite-temperature Thomas-Fermi (ftTF) model (Feynman *et al.*, 1949) and ftTF with second-order gradient corrections (ftSGA) (Perrot, 1979). Here we report first results of OF-DFT MD simulations for warm dense H with a pair of newly developed ftGGA free energy functionals [1] for the non-interacting kinetic energy and entropy. The equation of state from these new functionals shows much better agreement with the reference KS MD results than results from the ftTF and ftSGA models. Other issues, *e.g.* convergence of the OF self-consistent procedure, also will be discussed.

[1]. V.V. Karasiev, T. Sjostrom and S.B. Trickey, Phys. Rev. B **86**, 115101 (2012).

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