Abstract Submitted
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Orbital-free Molecular Dynamics Simulations to Characterize the Liquid-vapor Critical Point of Aluminum[1] DEBAJIT CHAKRABORTY, VALENTIN KARASIEV, QTP, Department of Physics, U. Florida, Gainesville, Fl, 32611, SAMUEL TRICKEY, QTP, Department of Physics and Chemistry, U. Florida, Gainesville, Fl, 32611 — Aluminum is frequently used in warm-dense matter (WDM) experiments. However, experimental diagnostic limitations make computational exploration of the Al liquid-vapor transition important[1]. The elevated temperaure and low-density make ab initio molecular dynamics (AIMD) with Kohn-Sham (KS) density functional theory (DFT) searches for the divergent compressibility extremely time consuming. Orbital free DFT (OFDFT) in principle is a cost-effective alternative. Here we report on calculations utilizing the PROFESS@QuantumEspresso interface [2] to explore suitable pseudo-potentials [3], the limitations of our wholly constraint-based VT84F [4] non-ineracting free-energy functional as exposed in the low-density regime, and possible extensions or extrapolations via tunable non-interacting free energy functionals [5]. [1] Atom. Proc. Plasmas **CP-1161** K. B. Fournier ed. (2009); [2] Comput. Phys. Commun. **185**, 3240 (2014); [3] J. Phys.: Condens. Matter **2**, 351 (1990); [4] Phys. Rev. B **88**, 161108(R) (2013); [5] "Tunable non-interacting free-energy functionals", V.V. Karasiev {unpublished}

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