Abstract Submitted
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**Tunable non-interacting free-energy functionals: development and applications to low-density aluminum**[1] SAMUEL TRICKEY, VALENTIN KARASIEV, Physics and QTP, Univ. Florida — We introduce the concept of tunable orbital-free non-interacting free-energy density functionals and present a generalized gradient approximation (GGA) with a subset of parameters defined from constraints and a few free parameters. Those free parameters are tuned to reproduce reference Kohn-Sham (KS) static-lattice pressures for Al at T=8 kK for bulk densities between 0.6 and 2 g/cm$^3$. The tuned functional then is used in OF molecular dynamics (MD) simulations [1] for Al with densities between 0.1 and 2 g/cm$^3$ and T between 6 and 50 kK to calculate the equation of state and generate configurations for electrical conductivity calculations [2]. The tunable functional produces accurate results. Computationally it is very effective especially at elevated temperature. Kohn-Shiam calculations for such low densities are affordable only up to T=10 kK, while other OF approximations, including two-point functionals, fail badly in that regime. 1. V.V. Karasiev, T. Sjostrom, and S.B. Trickey, Comput. Phys. Commun. 185, 3240 (2014). 2. V.V. Karasiev, L. Calderín, and S.B. Trickey, Phys. Rev. E 93, 063207 (2016).

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