Orbital-free molecular dynamics: application to hydrogen and deuterium under extreme conditions

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The computational and theoretical description of matter under extreme conditions, such as warm dense matter (WDM), is a non trivial task. Presently, the standard computational approach to WDM is a combination of the Kohn-Sham (KS) finite-temperature density functional theory (DFT) for the electrons and classical molecular dynamics (MD) for the ions. At high temperature (typically a few hundred kK) numerical solution of the system of thousands of coupled KS equations becomes an intractable task. 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 [1] and ftTF with gradient corrections usually truncated at second order (ftSGA) [2-4]. Here we report first results of OF-DFT MD simulations for warm dense hydrogen and deuterium with a pair of newly developed finite-temperature generalized gradient approximation (ftGGA) free energy functionals [5] for the non-interacting kinetic energy and entropy. The equation of state from the new Karasiev-Sjostrom-Trickey (KST2) functional (see Ref. [5] for details) is much closer to the reference KS MD results than results from other finite-temperature orbital-free models. Other issues, *e.g.* convergence of the orbital-free self-consistent procedure, also will be discussed.

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