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Properties of hot dense plasmas by Orbital-Free Molecular Dynamics JEAN CLEROUIN, CEA, DAM, DIF — During the last decade DFT calculations have been successfully applied to the WDM regime. To overcome the limitations of DFT in temperature and density we propose to return to the very basis of DFT by using an "only on the density" formulation of the electronic kinetic energy, essentially captured by the finite temperature formulation of the Thomas-Fermi theory. High temperatures (up to few KeV) and high densities (up to $10\times\rho_0$) systems can be addressed by orbital free molecular dynamics simulations (OFMD) at the expense of a fine description of atomic properties such as binding properties. Thanks to an efficient numerical scheme, up to thousands of particles can be propagated giving accurate static and dynamical properties without any assumptions on the ionization state or on the screening of interactions. Simulations of hydrogen and iron up to 5 keV and boron up to 10 times the normal density were performed. Very dissymmetrical mixtures can be also treated without difficulties. More recently, this method has been applied to hydrogen at high density (up to 160 g/cc) and high temperature (up to 1 KeV) to generate long trajectories for a later computation of the thermal conductivity with classical DFT. This method bridges the gap between quantum and classical molecular dynamics in the field of hot-dense plasmas and could be also used as a platform to include more physics such as nuclear reactions or interaction with a radiative field.

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