

Abstract Submitted
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Yukawa Monte Carlo (YMC) and Orbital Free Molecular Dynamics (OFMD) approaches for the eos of warm dense iron plasma DOMINIQUE GILLES, CEA/DSM/IRFU/SAP, FLAVIEN LAMBERT, JEAN CLEROUIN, CEA/DAM/DIF — Yukawa Monte Carlo and Molecular Dynamics simulations are powerful techniques extensively used to compute plasma properties such as EOS or transport coefficients, but are limited to applications where the linear electronic screening assumption is valid (1). Recently we have shown that a modified scheme using density functional theory with a Thomas-Fermi kinetic energy functional for the electrons (OFMD) may be well suited to perform MD simulations at high densities and temperature, without any assumption on the electronic screening (2). For selected iron plasma conditions representative of warm and dense matter, we shall compare pressure results calculated using YMC and OFMD codes and QEOS (3) and Sesame EOS models (4) and discuss the influence of keys parameters, like ionization in Yukawa theory.

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