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Simulation of the Correlated Electron Plasma in the Warm Dense Matter Regime by Restricted Path-Integral Molecular Dynamics[1] VIVEK KAPILA, University of Florida, PIERRE DEYMIER, University of Arizona, KEITH RUNGE, University of Florida — Warm dense matter (WDM) can be characterized by electron temperatures of a few eV and densities an order of magnitude or more beyond ambient. This regime currently lacks any adequate highly developed class of simulation methods. Recent developments in orbital-free Density Functional Theory (ofDFT) aim to provide such a simulation method, however, little benchmark information is available on temperature and pressure dependence of simple but realistic models in WDM regime. The present work aims to fill this critical gap using the restricted path-integral molecular dynamics (rPIMD) method. Within the discrete path integral representation, electrons are described as harmonic necklaces, while, quantum exchange takes the form of cross linking between electron necklaces. The fermion sign problem is addressed by restricting the density matrix to positive values and a molecular dynamics algorithm is employed to sample phase space. Here, we focus on the behavior of strongly correlated electron plasmas under WDM conditions. We compute the kinetic and potential energies and compare them to those obtained with the ofDFT method.

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