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Restricted Path-Integral Molecular Dynamics for Simulating the Correlated Electron Plasma in Warm Dense Matter[1] VIVEK KAPILA, University of Florida, PIERRE DEYMIER, University of Arizona, KEITH RUNGE, University of Florida — Several areas of study including heavy ion beam, large scale laser, and high pressure or Thomson scattering studies necessitate a fundamental understanding of warm dense matter (WDM) i.e. matter at high temperature and high density. The WDM regime, however, lacks any adequate highly developed class of simulation methods. Recent progress to address this deficit has been the development of orbital-free Density Functional Theory (ofDFT). However, scant 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. 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. The 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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