Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Simulation of the Warm-Dense Homogeneous Electron Gas[1] ETHAN BROWN, DAVID CEPERLEY, University of Illinois at Urbana-Champaign, JONATHAN DUBOIS, Lawrence Livermore National Laboratory — Warm-dense matter (WDM), where both the Coulomb coupling parameter ($\Gamma \equiv q^2/(r_s k_B T)$) and the electron degeneracy parameter ($\Theta \equiv k_B T/\epsilon_F$) are approximately unity, exists in systems as disparate as planetary interiors and along the pathway to inertial confinement fusion. Attempts to characterize this regime through the use of Density Functional Theory (DFT) require an accurate equation of state. Here we present results for a first-principles simulation of the homogeneous electron gas (HEG) in the warm-dense regime through Restricted Path Integral Monte Carlo (RPIMC). These results could be used as a benchmark for improved functionals, as well as input for orbital-free DFT formulations.

[1]DOE DE-F652-06NA26170

Ethan Brown
University of Illinois at Urbana-Champaign

Date submitted: 10 Nov 2011 Electronic form version 1.4