Abstract Submitted
for the DPP11 Meeting of
The American Physical Society

Path Integral Monte Carlo and Density Functional Molecular Dynamics Simulations of Warm Dense Matter BURKHARD MILITZER, KEVIN DRIVER, University of California, Berkeley — We analyze the applicability of two first-principles simulation techniques, path integral Monte Carlo (PIMC) and density functional molecular dynamics (DFT-MD), to study the regime of warm dense matter. We discuss the advantages as well as the limitations of each method and propose directions for future development. Results for dense, liquid helium, where both methods have been applied [1-3], demonstrate the range of each method's applicability. Comparison of the equations of state from simulations with analytical theories and free energy models show that DFT is useful for temperatures below 100000 K and then PIMC provides accurate results for all higher temperatures. We characterize the structure of the liquid in terms of pair correlation functions and study the closure of the band gap with increasing density and temperature. Finally, we discuss simulations of heavier elements and demonstrate the reliability are both methods in such cases with preliminary results.

[1] B. Militzer, Phys. Rev. Lett. 97 (2006) 175501.
[2] B. Militzer, Phys. Rev. B 79 (2009) 106407.
[3] B. Militzer, J Phys. A 42 (2009) 214001.

Burkhard Militzer
University of California, Berkeley

Date submitted: 27 Jul 2011 Electronic form version 1.4