

Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Path Integral Simulations of Heavy, Warm Dense Matter¹ KEVIN DRIVER, BURKHARD MILITZER, University of California, Berkeley — We develop an all-electron path integral Monte Carlo (PIMC) method for warm dense matter composed of elements with core electrons. For several second- and third-row elements, PIMC pressures, internal energies, and pair-correlation functions compare well with density functional theory molecular dynamics (DFT-MD) at low temperatures and enable the construction of coherent equations of state over a wide range of temperatures and densities. Details of the method and results will be discussed.

¹Funding provided by the NSF (DMS-1025370). Computational resources provided by the National Center for Atmospheric Research and Lawrence Berkeley National Laboratory.

Kevin Driver
University of California, Berkeley

Date submitted: 07 Nov 2012

Electronic form version 1.4