Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

First-principles equation of state and electronic properties of warm dense oxygen SHUAI ZHANG, KEVIN DRIVER, FRANOIS SOUBIRAN, BURKHARD MILITZER, University of California, Berkeley — We perform all-electron path integral Monte Carlo (PIMC) and density functional theory molecular dynamics (DFT-MD) calculations to explore warm dense matter states of oxygen. Our simulations cover a wide density-temperature range of 1-100 g cmˆ{−3}and 10ˆ4–10ˆ9 K. By combining results from PIMC and DFT-MD, we are able to compute pressures and internal energies from first-principles at all temperatures and provide a coherent equation of state. We compare our first-principles calculations with analytic equations of state, which tend to agree for temperatures above 8 x 10ˆ6 K. Pair-correlation functions and the electronic density of states reveal an evolving plasma structure and ionization process that is driven by temperature and density. As we increase the density at constant temperature, we find that the ionization fraction of the 1s state decreases while the other electronic states move towards the continuum. Finally, the computed shock Hugoniot curves show an increase in compression as the first and second shells are ionized. This work is funded by the DOE (DE-SC0010517).

Shuai Zhang
Univ of California - Berkeley

Date submitted: 08 Nov 2015 Electronic form version 1.4