Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Theoretical Investigation of Differing Ion and Electron Temperatures in Hydrogen[1] KEITH RUNGE, VALENTIN KARASIEV, Department of Physics, University of Florida, PIERRE DEYMIER, Materials Science and Engineering, University of Arizona — Andrew Ng [1] has reported experimental results for silicon and gold in warm, dense matter conditions that have been modeled by use of distinct temperatures for the ions and electrons. Here we investigate the implications of such differing ion and electron temperatures for hydrogen using path-integral molecular dynamics (PIMD) for protons which interact with electrons descibed by orbital-free density functional theory (OF-DFT). Temperatures ranging from room temperature to many kilokelvin are considered for the protons, while the electron temperatures are fixed in the kilokelvin range. Recent advances [2] in OF-DFT not only allow for faster generation of first principles forces but also include the effects of temperature on the electron density. Comparisons are made with classical molecular dynamics to allow us to quantify the quantum nuclear effects captured by PIMD.

[1] A. Ng, Int. J. Quantum Chem., 112, 150 (2012).
[2] V. V. Karasiev, D. Chakraborty, O. A. Shukruto, and S. B. Trickey, Phys. Rev. B 88, 161108(R) (2013).

[1]Work supported by U.S. Dept. of Energy, grant DE-SC0002139.

Keith Runge
Department of Physics, University of Florida

Date submitted: 11 Nov 2014 Electronic form version 1.4