Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Path Integral Molecular Dynamics for Hydrogen with Orbital-Free Density Functional Theory[1] KEITH RUNGE, VALENTIN KARASIEV, University of Florida, Gainesville, FL, PIERRE DEYMIER, University of Arizona, Tucson, AZ — The computational bottleneck for performing path-integral molecular dynamics (PIMD) for nuclei on a first principles electronic potential energy surface has been the speed with which forces from the electrons can be generated. Recent advances [A] in orbital-free density functional theory (OF-DFT) not only allow for faster generation of first principles forces but also include the effects of temperature on the electron density. We will present results of calculations on hydrogen in warm dense matter conditions where the protons are described by PIMD and the electrons by OF-DFT. [A] 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

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Date submitted: 14 Nov 2013 Electronic form version 1.4