Abstract Submitted
for the FWS19 Meeting of
The American Physical Society

Non-Adiabatic Molecular Dynamic Simulations of Warm Dense Matter[1] WILLIAM ANGERMEIER, RYAN DAVIS, REBEKAH HERMSMEIER, THOMAS WHITE, University of Nevada, Reno — The state and evolution of methane-rich planets, such as Uranus and Neptune, are determined by the properties of the dense and compressed matter in the planet interior. This compressed state, known as warm dense matter (WDM), is typically defined by temperatures of a few electron volts and densities comparable with those of solids. Recent experiments have suggested that non-adiabatic models that go beyond the Born-Oppenheimer approximation are necessary to describe such systems. We employ Wave Packet Molecular Dynamics(WPMD), a technique where the nuclei are treated classically, and the electrons are described as spherical Gaussian wave packets. In order to simulate large systems we use Electron Force Field(EFF) WPMD. EFF utilizes a Hartree product for the electron wavefunction and adds a correction term to the energy to account for Pauli exclusion. We benchmark EFF against orbital-free density functional theory across a broad range of phase space and, where available, experimental results. We show that the approximations within EFF breakdown at the highest densities. In order to extend the region of applicability, we begin to address two of the largest shortcomings of the EFF method, namely improvements to the approximation for the exchange energy and a more physical basis set.

[1]U.S. Department of Energy, Office of Science, Office of Fusion Energy Science under Award Number DE-SC0019268

William Angermeier
University of Nevada, Reno

Date submitted: 27 Sep 2019 Electronic form version 1.4