Abstract Submitted
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**Ion Modes in Dense Ionized Plasmas through Non-Adiabatic Molecular Dynamics**[1] WILLIAM ANGERMEIER, RYAN DAVIS, REBEKAH HERMSMEIER, THOMAS WHITE, University of Nevada, Reno — We perform non-adiabatic simulations of warm dense aluminum based on the electron-force field (EFF) variant of wave-packet molecular dynamics (WPMD) [1]. Comparison of the ion-ion structure factor and dispersion relation with density functional theory (DFT) is used to validate the technique across a range of temperatures and densities spanning the warm dense matter regime. At 3.5eV and 5.2 g/cm$^3$ we find a dispersion relation in close agreement with the more robust and adiabatic Kohn-Sham DFT. However, the approximations within EFF begin to breakdown at higher densities. To extend the region of applicability we suggest two improvements to the EFF model: (1) Improved approximation of the exchange and correlation energy and (2) a more physical basis set [2, 3].

1. A. Jaramillo-Botero et al. J.Comput. Chem. 32, 497 (2011).

2. R. A. Davis, W. A. Angermeier, R. Hermsmeier, and T. G. White. 2020. doi: ArXivID:2003.05566.

3. H. Xiao et al., Mechanics of Materials 90, 243–252 (2015).

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