The Summer Undergraduate Research Fellowship (SURF) Symposium
6 August 2015
Purdue University, West Lafayette, Indiana, USA

Quantum Molecular Dynamics Modeling of Warm Dense Matter

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ABSTRACT

Warm dense matter is attracting a lot of attention in the scientific community, due to its formation during intense laser-matter interaction and inertial confinement fusion. However, there is no accurate solution to mapping out the thermodynamic properties of warm dense matter. Experimental data are also incredibly scarce making computational models an incredibly useful tool. This paper provides equation of state (EOS) data for aluminum at specific densities within the warm dense matter regime. The EOS data were calculated using quantum molecular dynamics, which was performed by the computational package QuatumEspresso. EOS were determined by collecting and recording pressure after achieving equilibrium at a constant temperature and density. EOS data are plotted as a phase diagram. We found QuantumEspresso to be an accurate tool for predicting thermodynamic properties of WDM. Future research can be expanded to other materials and elements. The additional data on different materials can help other researchers to find trends and accurate EOS for warm dense matter.

KEYWORDS

Warm Dense Matter, Equations of State, Phase Diagram, Aluminum,