Density-Functional-Theory–Based Equation-of-State Table of Beryllium for Inertial Confinement Fusion Applications

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Based on density-functional-theory (DFT) calculations, we have established a wide-range beryllium EOS table of density $\rho = 0.001$ to $\rho = 500$ g/cm$^3$ and temperature $T = 2000$ to $10^8$ K.

The first-principles equation-of-state (FPEOS) table is in good agreement with the widely used SESAME EOS table (SESAME 2023), but shows a 10% difference in maximum compressibility from Purgatorio.

By implementing the FPEOS table into our hydrocodes, we show that the FPEOS simulation predicts a higher neutron yield (~15%) compared to the simulation using the SESAME 2023 simulations.
Combining orbital-based DFT and orbital-free molecular dynamics (OFMD), we have investigated wide-ranged EOS tables of beryllium

- Previous FPEOS studies on D₂, CH, and Si show a significant difference from SESAME 2023
- As an inertial confinement fusion (ICF) ablator, accurate properties of beryllium under such extreme conditions are essential for designs
- Theoretical EOS models may not provide an accurate EOS in the warm-dense-matter (WDM) regime, where both strongly coupled (Γ > 1) and degeneracy effects (θ < 1) are important*
- Quantum molecular dynamics (QMD),* based on DFT, has proven to work well for EOS calculations**

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The FPEOS of beryllium has been calculated for densities and temperatures from $\rho = 0.001\ \text{g/cm}^3$ to $\rho = 500\ \text{g/cm}^3$ and $T = 2000\ \text{K}$ to $10^8\ \text{K}$

The calculated principal shock Hugoniot of beryllium from FPEOS has been compared with other theoretical models and experiments. The FPEOS Hugoniot pressure of beryllium is in good agreement (within 10%) with the widely used SESAME model (SESAME 2023) in the low-compression-ratio region; the pressure differences can be up to 30% in the high-compression region.
The off-Hugoniot equation of state is compared between FPEOS and SESAME at certain densities
In the WDM regime the difference between FPEOS and SESAME 2023 can reach a maximum of 20%
The implication of Be FPEOS for ICF designs has been examined.

For DT, two gas simulations used the same FPEOS table and the first-principles opacity table.
The FPEOS simulation predicted ~15% higher neutron yield than the SESAME simulation.

This small difference between FPEOS and SESAME in hydro simulations is consistent with their good agreement with the Hugoniot.
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An accurate equation-of-state (EOS) table of beryllium has been built from first-principles calculations.