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Equations of State for Mixtures: Results from DFT Simulations of Xenon/Ethane Mixtures Compared to High Accuracy Validation Experiments on Z

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We report a computational and validation study of equation of state (EOS) properties of liquid / dense plasma mixtures of xenon and ethane to explore and to illustrate the physics of the molecular scale mixing of light elements with heavy elements. Accurate EOS models are crucial to achieve high-fidelity hydrodynamics simulations of many high-energy-density phenomena such as inertial confinement fusion and strong shock waves. While the EOS is often tabulated for separate species, the equation of state for arbitrary mixtures is generally not available, requiring properties of the mixture to be approximated by combining physical properties of the pure systems. The main goal of this study is to access how accurate this approximation is under shock conditions. Density functional theory molecular dynamics (DFT-MD) at elevated-temperature and pressure is used to assess the thermodynamics of the xenon-ethane mixture. The simulations are unbiased as to elemental species and therefore provide comparable accuracy when describing total energies, pressures, and other physical properties of mixtures as they do for pure systems. In addition, we have performed shock compression experiments using the Sandia Z-accelerator on pure xenon, ethane, and various mixture ratios thereof. The Hugoniot results are compared to the DFT-MD results and the predictions of different rules for combing EOS tables. The DFT-based simulation results compare well with the experimental points, and it is found that a mixing rule based on pressure equilibration performs reliably well for the mixtures considered.

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