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Ethane-xenon mixtures under shock conditions DAWN FLICKER, RUDOLPH MAGYAR, SETH ROOT, KYLE COCHRANE, THOMAS MATTSSON, Sandia National Laboratories — Mixtures of light and heavy elements arise in inertial confinement fusion and planetary science. We present results on the physics of molecular scale mixing through a validation study of equation of state (EOS) properties. Density functional theory molecular dynamics (DFT/QMD) at elevated-temperature and pressure is used to obtain the properties of pure xenon, ethane, and various compressed mixture compositions along their principal Hugoniots. To validate the QMD simulations, we performed high-precision shock compression experiments using Sandia's Z-Machine. A bond tracking analysis of the simulations correlates the sharp rise in the Hugoniot curve with completion of dissociation in ethane. DFT-based simulation results compare well with experimental data and are used to provide insight into the dissociation as a function of mixture composition. Interestingly, we find that the compression ratio for complete dissociation is similar for ethane, Xe-ethane, polymethyl-pentene, and polystyrene, suggesting that a limiting compression exists for C-C bonded systems. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Company, Security Administration under contract DE-AC04-94AL85000.

Dawn Flicker
Sandia National Laboratories

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