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Equation of state of mixtures: density functional theory (DFT) simulations and experiments on Sandia's Z machine R.J. MAGYAR, S. ROOT, T.A. HAILL, D.G. SCHROEN, T.R. MATTSSON, D.G. FLICKER, Sandia National Laboratories, SANDIA NATIONAL LABORATORIES COLLABORATION — Mixtures of materials are expected to behave quite differently from their isolated constituents, particularly when the constituents atomic numbers differ significantly. To investigate the mixture behavior, we performed density functional theory (DFT) calculations on xenon/hydrogen, xenon/ethane, and platinum/hydrocarbon mixtures. In addition, we performed shock compression experiments on platinum-doped hydrocarbon foams up to 480 GPa using the Sandia Z - accelerator. Since the DFT simulations treat electrons and nuclei generically, simulations of pure and mix systems are expected to be of comparable accuracy. The DFT and experimental results are compared to hydrodynamic simulations using different mixing models in the equation of state. The role of de-mixing and the relative contributions of the enthalpy of mixing are explored. Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of the Lockheed Martin company, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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