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Equations of state of ablator materials[1] SHUAI ZHANG, Lawrence Livermore Natl Lab, BURKHARD MILITZER, University of California, Berkeley, HEATHER WHITLEY, Lawrence Livermore National Laboratory — We use path integral Monte Carlo (PIMC) and density functional theory molecular dynamics (DFT-MD) to calculate equations of state (EOS) of a series of ablator materials (CHx, B, BN, and B4C) over a wide range of temperatures ($0.1 10^4$ eV) and densities (0.01100 g/cc). We demonstrate remarkable thermodynamic consistency between the EOSs from DFT-MD calculations using different exchange-correlation functionals and those derived from PIMC with free-particle nodes. This provides strong evidence for the applicability accuracy of PIMC and DFT-MD to predict the properties of warm dense matter. Our predictions constrain the EOS to better than 4%, with the largest uncertainties occurring at 10^6 K where K shell starts to ionize. We study the ionic and electronic structure over a wide range of temperature, density and composition. We find the linear mixing approximation to be valid with high accuracy. We make predictions for the effects of oxygen content and C:H ratio on shock compression. We conclude by discussing other simulation methodologies and reviewing existing Hugoniot experiments across the GPa-TPa warm dense regime. By combining experimental and theoretical EOS data we construct consistent EOS tables for inertial confinement fusion and high-energy-density simulations.

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