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Wide-range equations of state of carbon and boron materials from first principles[1] SHUAI ZHANG[2], HEATHER WHITLEY, LORIN BENEDICT, LIN YANG, KYLE CASPERSEN, JIM GAFFNEY, MARKUS DAENE, JOHN PASK, PHILIP STERNE, TADASHI OGITSU, AMY LAZICKI, MICHELLE MARSHALL, DAMIAN SWIFT, Lawrence Livermore Natl Lab, BURKHARD MILITZER, University of California, Berkeley, SUXING HU, Laboratory for Laser Energetics, University of Rochester, WALTER JOHNSON, University of Notre Dame — Using several independent approaches (path integral Monte Carlo, density functional theory, and activity expansion), we performed extensive investigation providing the theoretical benchmark for the equations of state (EOS) of a series of low-Z materials (CHx, B, BN, and B4C) over a wide range of temperatures (0.1-1e4 eV) and densities (0.01-100 g/cc). Across the warm-dense regime, our predictions show remarkable consistency with experimental data and constrain the EOS to better than 4%, with the largest uncertainties occurring at 1e6 K and 1 Gbar where K shell ionization occurs. Constrained by our first-principles data, we made improved EOS models to be used for the design and interpretation of high-energy-density and inertial confinement fusion experiments. We also discuss the strengths and weaknesses of empirical approaches such as the ideal-mixing approximation and the Arrhenius relation, as well as structural complexities during shock compression. (LLNL-ABS-780064)

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