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Construction of a multi-phase equation of state for carbon at extreme pressures[1] ALFREDO A. CORREA, University of California at Berkeley and Lawrence Livermore National Laboratory, LORIN X. BENEDICT, Lawrence Livermore National Laboratory, STANIMIR A. BONEV, Dalhousie University, Halifax, Canada, DAVID A. YOUNG, Lawrence Livermore National Laboratory, ERIC SCHWEGLER, Livermore National Laboratory — We describe the construction of a multi-phase equation of state for carbon at extreme pressures that is based on the results of first principles electronic structure calculations. Two solid phases (diamond, BC8) and the liquid are considered. Solid-phase free energies are built from a knowledge of cold curve and phonon calculations, together with first principles molecular dynamics calculations of the equation of state itself to extract anharmonic terms. The liquid free energy is constructed from a combination of molecular dynamics calculations and constraints determined from previously calculated melt curves, assuming a simple solid-like free energy model. The resulting equation of state is extended to more extreme densities and temperatures with a plasma-based free energy model. Comparisons to available experimental results are discussed.

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