Abstract Submitted
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A multiphase equation of state for carbon addressing high pressures and temperatures[1] LORIN BENEDICT, Lawrence Livermore National Laboratory, KEVIN P. DRIVER, University of California at Berkeley, SEBASTIEN HAMEL, Lawrence Livermore National Laboratory, BURKHARD MILITZER, University of California at Berkeley, TINGTING QI, ALFREDO A. CORREA, ERIC SCHWEGLER, Lawrence Livermore National Laboratory — We present a 5-phase equation of state (EOS) for elemental carbon. The phases considered are: diamond, BC8, simple-cubic, simple-hexagonal, and the liquid/plasma state. Free energy models for the various phases are constrained by Density Functional theory (DFT) and path integral quantum Monte Carlo calculations. The precise manner in which the ideal gas limit is reached is greatly constrained by both the highest temperature DFT data and the path integral data, forcing us to discard an ion-thermal model we had used previously in favor of a new one. Predictions are made for the principal Hugoniot and the room-temperature isotherm, and comparisons are made to recent experimental results.

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