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Carbon under extreme conditions: phase boundaries from first-principles theory ALFREDO A. CORREA, Physics Department, University of California, Berkeley, STANIMIR A. BONEV, Department of Physics, Dalhousie University, Halifax, GIULIA GALLI, Department of Chemistry, University of California, Davis — We present predictions of diamond and BC8 melting lines and their phase boundary in the solid phase, as obtained from first principles calculations. Maxima are found in both melting lines, with a triple point located at ~ 850 GPa and ~ 7400 K. Our results show that hot, compressed diamond is a semiconductor which undergoes metalization upon melting. On the contrary, in the stability range of BC8, an insulator to metal transition is likely to occur in the solid phase. Close to the diamond/ and BC8/liquid boundaries, molten carbon is a low-coordinated metal retaining some covalent character in its bonding up to extreme pressures. Our data provide constraints to the carbon equation of state, which is of critical importance to devise models of, e.g., Neptune, Uranus and white dwarf stars, as well as of extra-solar carbon planets. This work was performed under the auspices of the U.S. Dept. of Energy at the University of California/Lawrence Livermore National Laboratory under contract no. W-7405-Eng-48.

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