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First-principles molecular dynamics simulations of high-pressure phase diagram of carbon KIEN NGUYEN CONG, JONATHAN WILLMAN, ASHLEY WILLIAMS, University of South Florida, ANATOLY BELONOSHKO, Royal Institute of Technology, IVAN OLEYNIK, University of South Florida — Although high-pressure phase diagram of carbon at extreme temperatures and pressures has been in the focus of intensive experimental and theoretical studies, there still exist outstanding problems including disagreement between theoretical predictions and experiment. We present results of first-principles molecular dynamics simulations of thermodynamic properties of carbon at high temperatures and pressures, which are performed with the goal of constructing an accurate phase diagram of carbon. To address the issue of accuracy and reliability, a relatively large number of atoms is used for calculation of melting transitions (melt curve) as a function of pressure. Accurate Gibbs free energies are calculated using temperature dependent effective potential method. We specifically focus on important region of phase diagram where diamond exhibits a negative melting line slope at pressures above 500 GPa.

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