Local structure, thermodynamics, and melting of boron phosphide at high pressures by deep learning-driven ab initio simulations

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Boron phosphide (BP) is a (super)hard semiconductor constituted of light elements, which is promising for high demand applications at extreme conditions. We develop a deep machine learning potential (DP) for accurate atomistic simulations of the solid and liquid phases of BP as well as their transformations near the melting line. Our DP provides quantitative agreement with experimental and ab initio molecular dynamics data for structural and dynamic properties. The main contributions to structural changes at low pressures are made by the evolution of medium-range order in the B-subnetwork and, at high pressures, by the change of short-range order in the P-subnetwork. Such transformations exhibit an anomalous behavior of structural characteristics in the range of 12–15 GPa. DP-based simulations reveal that the $T_m(P)$ curve develops a maximum at $P = 13$ GPa, whereas experimental studies provide two separate branches of the melting curve, which demonstrate the opposite behavior [1].

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