

Abstract Submitted
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Computational studies of the boron carbide structure SANXI YAO,
Carnegie Mellon Univ — Boron carbide is a structure that exhibits a broad composition range, implying a degree of intrinsic substitutional disorder. While the observed symmetry is rhombohedral, the enthalpy minimizing structure has lower, monoclinic, symmetry. We apply compressive sensing to fit a pair interaction model to a database of structural energies. Utilizing histogram methods to analyze Monte Carlo simulations of this model, we investigate the symmetry-restoring phase transition that explains the observed rhombohedral symmetry at high temperatures.

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