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Molecular dynamics studies of Schottky and Frenkel defects in cubic boron nitride

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Abstract content
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Schottky and Frenkel defect energies in boron nitride are studied using the classical molecular dynamics. Tersoff potentials are used to enlighten the boron-nitrogen, boron-boron and nitrogen-nitrogen interactions in the bulk and defect structures. The formulation uses the NVT Evans ensemble to obtain the various defect energies. Boron and nitrogen vacancy defect energies relative to bulk boron nitride total energies are used to get more insight on cubic boron nitride as a strong material. The nature of Schottky and Frenkel defects in this material are discussed.

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