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Structural and mechanical properties of BP3N6

Using first-principles calculation, the structural and mechanical properties of BP3N6 which adopts an orthorhombic structure with space group Pna21 (no. 33), were determined at three different pressure values (0, 20 and 42.4 GPa). The nine independent elastic constants meet all necessary and sufficient conditions for mechanical stability criteria for an orthorhombic crystal. BP3N6 show strong resistance to volume change hence a potential low compressible material. The Vicker's hardness of BP3N6 was found to range between 49-51 GPa for different external pressures imposed on the crystal. These high values of Vicker's hardness imply that BP3N6 is potential superhard material.

Keywords

boron phosphorus nitride; DFT; Vickers hardness.

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