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Pressure Effect Study on the Electronic and Optical Properties of $B_xIn_{1-x}As$ Alloys Using DFT Calculation

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In order to extract structural and electronic properties of $B_xIn_{1-x}As$ ternary alloys and enrich the database of materials based on boron and indium, we have used full-potential augmented plane wave (FP-LAPW) method through the density function theory (DFT) and within generalized gradient approximation (GGA), local density approximation (LDA), and Tran–Blaha modified Becke–Johnson approximation (TB−mBJ). We have optimized the cohesive energy of our binary compound and ternary alloys versus volume of the unit cell firstly, and we have found that the optimum volume, lattice parameter, and the bulk modulus vary for different boron concentrations. Using DFT−mBJ calculations, we found that InAs possess direct band-gap energy and an indirect gap semiconductor for BAs and $B_{0.75}In_{0.25}As$. However, $B_{0.25}In_{0.75}As$ and $B_{0.5}In_{0.5}As$ ternary alloys have a metallic and semi metallic characters, respectively. We also studied the optical properties of our BAs and InAs binary and $B_{0.75}In_{0.25}As$ ternary semiconductors and their behaviors are also investigated under the application of hydrostatic pressure in a range of 0 to 25 GPa.

In summary, we conclude that the incorporation of boron atom in InAs increase its hardness and affects the band-gap energy considerably, and therefore provides a novel research perspective. We note that InAs binary compound loses its semiconductor character and becomes semi-metal at 5 GPa.

Keywords: InAs, BAs, $B_xIn_{1-x}As$, mBJ approximation.