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First-principles calculations of the structural, electronic and optical properties of $In_{1?x}B_xAs_yP_{1?y}$ quaternary alloys lattice matched to InP and BeS

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Abstract: The structural, electronic, and optical properties of the cubic $In_{1?x}B_xAs_yP_{1?y}$ quaternary alloys lattice matched to InP and BeS have been investigated by using the full-potential linearized augmented plane wave (FP-LAPW) method within the density functional theory (DFT). The generalized gradient approximation (GGA) of Wu and Cohen was used as the exchange correlation potential to calculate the structural and electronic properties. In addition, the alternative GGA proposed by Engel and Vosko and the modified Becke–Johnson potential are utilized to calculate the electronic properties. The computed structural and electronic properties of the binary compounds are in good agreement with the available experimental and theoretical data. For the alloys, non-linear variations of composition x and y with the lattice constant, bulk modulus, direct, indirect band gap, dielectric constant and refractive index are found. All the compounds are direct band gap excluding BP and BAs. The energy band gap of $In_{1?x}B_xAs_yP_{1?y}$ quaternary alloys lattice matched to InP and BeS substrates is computed. Finally, the band gap of our materials is less than 3.1 eV. Thus the $In_{1?x}B_xAs_yP_{1?y}$ quaternary alloys may possibly be used in visible light devices.

Keywords : FP-LAPW, DFT, In1?xBxAsyP1?y quaternary alloys, Lattice matched