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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.

1. Introduction

Semiconductors are tremendously important both technologically and economically [1–6]. The III–V and II–VI semiconductor alloys are promising candidates for many device applications such as high speed electronic and long wavelength photonic devices because their band gaps cover a wide spectral range [7]. Recently, the optoelectronic devices of III–V compounds have advantages over II–VI semiconductor devices due to some interesting applications in optical communication systems such as diodes laser, light-emitting diodes, photodetectors, electro-optic modulators and frequency mixing components [8–11]. The major goal of materials engineering is the ability to tune independently the band gap energy and the lattice constant in order to obtain the desired optical properties. One of the easiest methods to change artificially the properties of semiconductors is by forming the alloys; the adapt of two, three or four different binary compounds with different optical band gaps could lead to new semiconductor material with desired band gap and lattice constant over a continuous broad composition range. Hence, we noted in the last decade several researches that led to the development of new material systems based on the incorporation of boron into conventional III–V binary compounds and ternary alloys. These materials have a wide range of technological potentials in the

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