Structural, electronic properties of compounds AlAs, BAs and AlP, BP

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\textbf{Abstract.} We determine the structural, electronic properties of AlAs, BAs and AlP BP alloys using the full potential-linearized augmented plane wave method (FP-LAPW) within the density functional theory (DFT). The exchange-correlation potential is treated by the generalized gradient approximation (WC-GGA). The investigation on the effect of composition on lattice constant, bulk modulus and band gap shows not linear dependence on the composition. The ground state properties such as lattice constant, bulk modulus, pressure derivative of the bulk modulus are in good agreement with numerous experimental and theoretical data. For the electronic properties, we used the mBJ-LDA approximation. The bowing of the fundamental gap versus composition predicted on the composition is in a good agreement with experiment.

\textbf{Keywords:} FP-LAPW, DFT, Ternary alloys, bands structure, bowing gap and thermodynamic properties.

\section*{INTRODUCTION}

Semiconductor alloys, which are solid solutions of two or more semiconducting elements, have important technological applications, especially in the manufacture of electronic and electrooptical devices [1]. One of the easiest ways to change artificially the electronic and optical properties of semiconductors is by forming their alloys; it is then interesting to combine two different compounds with different optical band gaps and different rigidities in order to obtain a new material with intermediate properties. The advantage in mixed crystals between III–V compounds has been fully utilized for realization of optical devices [2]-[3].

In addition to their interesting properties, these materials possess some peculiar characteristics that we discuss and try to explain in the present work. Among these peculiar characteristics is the inverse role between the cation and the anion in terms of charge transfer and the new phase transition.

The calculations were performed using full-potential (linear) augmented plane wave (FP-LAPW) method [4]-[5]-[6] within the framework of density functional theory (DFT) [7], [8] as implemented in WIEN2K [9] code. For structural properties the exchange-correlation potential was calculated using the generalized gradient approximation (GGA) in the new form (WC) proposed by Wu and Cohen [10] which is an improved form of the most popular Perdew-Burke-Enrzerhof (PBE) GGA [11]. In addition and for electronic properties only, we also applied the modified Becke-Johnson (mBJ) [12] scheme.