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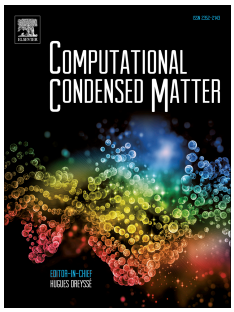

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Structural, electronic and optical properties of InP under presure: An ab-initio study

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Abstract. In this paper, we presented an ab-initio study of the structural, electronic and optical properties of the binary compound of indium phosphide (InP). This material is widely used in the field of optoelectronics and microelectronics fast. Our calculations were made by the method of augmented plane wave (FP-LAPW), based on the density functional theory (DFT) and implemented in the calculation code Wien2k. This calculus of the electronic band, structure and optical properties were performed using local-density approximation (LDA), generalized gradient approximation (GGA), and a combination of modified Becke—Johnson exchange potential plus LDA and GGA (mBJ + LDA/GGA) for exchange–correlation potential. We find in our calculations, the usual trends, that the (GGA) unlike LDA overestimates the lattice parameter and underestimates the bulk modulus. The phase transitions for this material from structure B3 to structures Imm2, B8-1, B10 and B2 are possible under low pressures and The calculation of the density of state gives a detailed explanation of the contribution of the different orbitals.

Keywords: DFT, FP-LAPW, mBJ+LDA/GGA, InP, Pressure.

1. Introduction

It's very interesting optical features make the InP a very popular material in the field of optoelectronics and fast microelectronics. It is used in the manufacturing of devices such as, diodes (LED, laser, electroluminescent), transistors (WT, FET and field effect) and optical amplifiers. The realization of InP heterojunction bipolar transistors is an important issue in the development of high-speed optical fiber communication systems (20 to 40 Gbit/s) [1]. In fact, the laser diodes and the photo-detectors made from InP are compatible with the wavelengths used for this type of transmission (1.3 to 1.55 μm) and obtaining good quality TBH InP would allow monolithic integration of optoelectronic devices based on InP.
Precise measurements of the electronic band configuration and its dependent optical characteristics are required for the optimal device operation.X-ray photoemission spectroscopy was used in the InP study by Ley et al. [2]. Aspnes and Stunda [3] measured the dielectric function of InP with that of other III-V semiconductors by spectroscopic ellipsometry between 1.5 and 6.0 eV.

It should be mentioned here that the band gap values calculated in this work are in close agreement with the experimental results compared to other functional exchange correlations. The difference between these results and the other reported results is the first use of the modified "Becke Johnson Potential" technique (mBJ) to study this compound. The mBJ is known to overcome the problem of underestimation of gaps, in the case of local density approximation (LDA) [4] and generalized gradient approximation (GGA) [5]. Several studies have been conducted using the mBJ potential to calculate the electronic properties of different families of solids. These studies support the fact that the method provides significantly improved and accurate bandwidth energy values for a wide range of different materials. [6-7].

This paper is organised as follows. In Section 2, we describe the calculation method used in this work. In section 3, we present the calculated structural, electronic and optical properties. Finally, we summarize the results in section 4.

2. Methods

We performed our calculations using FP-LAPW as part of DFT [8] using Wien2k code [9]. MBJ is used to minimize the shortcomings of the LDA and GGA approximations in terms of poor evaluation of the band gap value. The mBJ-GGA V_{xc} potential [10] uses the mBJ exchange potential plus the GGA correlation potential and performs the band gap calculation accurately, similar to the computationally expensive GW calculations. This method provides the band gap almost equal to the experimental values. The wave functions cut-off were considered K_{max}=8/RMT in the interstitial spaces, where RMT is the smallest atomic muffin-tin sphere radius and Kmax is the largest K vector in the plane wave extension. The valence wave functions inside the muffin-tin spheres were expanded up to l_{max}=10, whereas the charge density was Fourier expanded up to G_{max}=14(a.u). The self-consistent calculations are regarded to be converged when the total energy of the

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