STRUCTURAL, ELECTRONIC AND OPTICAL PROPERTIES OF $\text{Sc}_x\text{Ga}_{1-x}\text{P}$ ALLOYS AN: AB INITIO STUDY

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Article Info	Abstract
<p>Received: 02.08.2021 Accepted: 21.10.2021</p> <p>Keywords: FP-LAPW, $\text{Sc}_x\text{Ga}_{1-x}\text{P}$, PBE-GGA, TB-mBJ, ab-initio study</p>	<p>The structural, electronic and optical properties of the of $\text{Sc}_x\text{Ga}_{1-x}\text{P}$ alloys have been investigated by using the full-potential plane-wave FP-LAPW method as implemented in the Wien2k code. The exchange-correlation (XC) energy of electrons was treated using the Perdew-Burke-Ernzerhof parametrization (PBE-GGA), and the Tran-Blaha modified Beck-Johnson potential (TB-mBJ). The lattice constant and the bulk modulus have been calculated and analyzed where a deviation from Végard's law is observed for both.</p> <p>The calculation of the band structure of binary GaP shows that there is an indirect gap of 2.27 eV, while for the $\text{Sc}_x\text{Ga}_{1-x}\text{P}$ compounds there are direct gaps with values of 1.91 eV, 1, 39 eV, 2.04 eV and 1.849 eV for $x = 0.25, 0.5, 0, 75$ and 1, respectively.</p> <p>At ambient pressure, the refractive index and the dielectric constant are in good agreement with the experimental results. The extinction coefficient does not begin to increase until a threshold, which represents the optical gap. This threshold is equal to 1.224 eV and it starts to increase to reach a maximum at an energy of 3.551 eV.</p>

1.Introduction

III–V compound semiconductors are of practical interest and the range of technical applications for these semiconductors is extremely wide. Knowledge of these binary and ternary phosphide compounds remains scarce. Recently, the motivation to study their

properties has been due to their great importance in technological applications [1], whether for technological purposes or at a purely fundamental level.

Their technological applications in electronics and optoelectronics are numerous, such as lasers and light emitting diodes, photodetectors, CD and DVD players, remote controls, cell phones and other devices, including fiber optic telecommunications. There are studies in the literature that describe the behavior of binary phosphides as semiconductors [2].

GaP is a III-V compound, which has physical properties of interest for the development of optoelectronics [2]. It crystallizes in the (ZnS) structure (space group F43 m) with a lattice constant of 5.45 Å [2.3]. It exhibits a phase transition to phase (NaCl) (space group Fm3 m) at a transition pressure of 26 GPa [4.5]. GaP is an indirect gap semiconductor with a band gap energy of 2.35 eV [2.3], and its applications have led to the manufacture of green, red and orange light-emitting diodes (LEDs) [6.7]. It is also used as an active material for visible LEDs [1,9]. Experimental studies seek to improve the physical properties and luminescence of GaP in the manufacture of LEDs by doping it with low concentrations of nitrogen [8].

Scandium phosphide (ScP) is a III-phosphide binary, experimental X-ray studies have shown that scandium phosphide crystallizes in the NaCl phase with a lattice parameter of 5.31 Å [9,10].

It could undergo a transition from the sodium chloride (NaCl) phase to the cesium chloride (CsCl) phase at a transition pressure of 245.6 GPa [11].

A theoretical study has predicted that it has a metallic structure in the NaCl [6] and Zinc-blende [7] phases.

Combining these two materials using growth techniques can result in new materials with the same properties. Among these ternary materials that crystallized in the same structure and produced very similar lattice parameters is the $\text{Sc}_x\text{Ga}_{1-x}\text{P}$ alloy which characterized by a stoichiometric modulus of x.

Calculations on the properties of compounds containing scandium have been reported in some theoretical work by S. Benalia et al. carried out an FP-LMTO study of the bandgap of $\text{Sc}_x\text{Ga}_{1-x}\text{P}$ and $\text{Sc}_x\text{Al}_{1-x}\text{P}$ [11]

Although, W. Celin-Mancera et al. have studied the electronic, elastic and thermodynamic properties of $\text{Sc}_x\text{Ga}_{1-x}\text{P}$ compounds by the FP-LAPW method [10]. However, S. Benalia et al have combined the resulting $\text{Sc}_x\text{Al}_{1-x}\text{P}$ and $\text{Sc}_x\text{Ga}_{1-x}\text{P}$ in layers to obtain new materials; $\text{Sc}_{0.25}\text{Ga}_{0.75}\text{P}/\text{Sc}_{0.5}\text{Ga}_{0.5}\text{P}$ and $\text{Sc}_{0.25}\text{Al}_{0.75}\text{P}/\text{Sc}_{0.5}\text{Ga}_{0.5}\text{P}$ super lattices [11].

Among the best known and most usable ab-initio methods is the linearized augmented plane wave (FP-LAPW) method used to calculate the physical properties of materials. It has remained by far the most widely used and most efficient for several years. Moreover, its advantage lies in the fact that it can process a large number of atoms. For this purpose, we have used first principle calculations to study the structural and electronic properties of the binary compounds ScP, GaP and the ternary alloy $\text{Sc}_x\text{Ga}_{1-x}\text{P}$ over a range of compositions ($0 \leq x \leq 1$). The objective of the work is the study of the structural, electronic and optical properties of the ternary alloy $\text{Sc}_x\text{Ga}_{1-x}\text{P}$.

Now, and after this introduction, we will briefly describe the method used and give the details of the calculation. Next, we will discuss in detail the results regarding the structural, electronic and optical properties of our ternary and finally, in the last section, we present the conclusion of our current work.

2. Computational details

The calculations we have performed on the Linearized Augmented Plane Wave (LAPW) method, which leads to the self-coherent resolution of the Kohn-Sham equations within the framework of the Density Functional Theory (DFT), as implemented in the WIEN2k code [13-15]. The exchange and correlation potential has been treated by different approximations, which are the generalized gradient (GGA) of the exchange potential of Perdew, Burke and Ernzerhof (PBE) [16] and Tran-Blaha modified Becke-Johnson exchange potential approximations (TB-mBJ) [17]. The reason why the different approximations were used to calculate the structural properties, was to enrich and compare the different results obtained.

It is taken into account that the GGA approach overestimates the lattice parameter and underestimates the gap energies, the values of the lattice parameter, the gap energies and the compression modulus calculated by the generalized gradient approximation parameterized of Perdew-Burke-Ernzerhof (PBE-GGA). However, all of the above approximations considerably underestimate the gap energies. Fortunately, the Tran-Blaha approximation based on the Becke-Johnson modified potential parameterized (TB-mBJ) by Koller et al [18, 19], which has been developed recently, in fact gives actually very satisfactory results with regard to the gaps.

The unit cell is divided into two regions, the first one is made up of spheres that do not overlap and are centered on each atom with radius RMT, the second one is the interstitial region. Wave functions, electron densities and potential are developed as a combination of

spherical harmonics multiplied by radial functions around atomic sites in Muffin-tin spheres with a cut-off radius $l_{\max} = 10$. However, they are Fourier series expanded in the interstitial region with a cut-off radius $R_{\text{MT}} \times k_{\max} = 8$, where R_{MT} is the smallest radius of the MT sphere and $k_{\max}$ is the plane wave cutoff. The values of the radii have been set at $R_{\text{MT}}(\text{Ga}) = 2.5$ a.u., $R_{\text{MT}}(\text{Sc}) = 2.32$ a.u and $R_{\text{MT}}(\text{P}) = 2.22$ a.u.

Structural optimization consists in determining the ground state. The iteration process is repeated until the total energy is stable at 10^{-5} Ry. The energy separating the valence states and the core states was taken equal to -9 Ry. The electronic valence configuration of the atoms used is: Ga ($4s^2 3d^{10} 4p^1$), Sc ($3d^1 4s^2$) and P ($3s^2 3p^3$).

3. Results and Discussions

3.1. Structural properties

First, we have calculated the structural properties of the binary compounds ScP in the NaCl phase under normal conditions and GaP in the ZnS phase which is their equilibrium phase using the generalized gradient approximation parameterized of Perdew-Burke-Ernzerhof (PBE-GGA) scheme. Next, the $\text{Sc}_x\text{Ga}_{1-x}\text{P}$ alloy was modeled to some of the compositions of $x = 0.25, 0.5$ and 0.75 . We have taken a conventional GaP cubic cell containing eight atoms, four Ga atoms and four P atoms. In this eight-atom model, the alloy $\text{Sc}_{0.25}\text{Ga}_{0.75}\text{P}$ is obtained by replacing an atom of Ga by an atom of Sc. The $\text{Sc}_{0.5}\text{Ga}_{0.5}\text{P}$ alloy is obtained by replacing two Ga atoms by two Sc atoms and finally for $\text{Sc}_{0.75}\text{Ga}_{0.25}\text{P}$ three Ga atoms must be replaced by three Sc atoms.

The different crystal structures used correspond to the different Sc% concentrations shown in fig 1.

We have calculated the change in total energy as a function of unit cell volume, and the resulting curve was fitted to Murnaghan's equation of state [20] to obtain the lattice constant a_0 , as well as the bulk modulus B and its derivative B' . Results are presented in Table 1 with the available theoretical and experimental data. The obtained values are in good agreement with the experimental data and even with the theoretical results of previous works.

Figure 1. The different crystal structures used correspond to the different Sc% concentrations.

Table 1. Calculated lattice parameter a_0 , bulk modulus B and its derivative B' for the binary ScP, GaP and for the ternary alloy $Sc_xGa_{1-x}P$ where $x = 0.25, 0.5$ and 0.75 compared to the experimental and theoretical data available.

Compound	a_0 (Å)	B (GPa)	B'	E_{coh} (eV)
GaP	5.52* 5.50 ^a 5.45 ^b	77.49* 76.41 ^a 91 ^d	4.81* 4.6 ^c	26,888*
Sc _{0.25} Ga _{0.75} P	5.66* 5.65 ^a 5.57 ^c	69.93* 67.68 ^a	4.38* 4.18 ^a	27,287*
Sc _{0.5} Ga _{0.5} P	5.78* 5.77 ^b	66.57* 63.96 ^d	4.17* 4.13 ^c	27,635*
Sc _{0.75} Ga _{0.25} P	5.87* 5.86 ^b	64.47* 63.02 ^a	3.98* 3.31 ^c	27,775*
ScP	5.94* 5.93 ^b	63.49* 63.93 ^d	3.51* 3.24 ^e	27,903*

*Present calculations

^a Ref. [2], ^b Ref. [21], ^c Ref. [23], ^d Ref. [3], ^e Ref. [12].

Figure 2. Composition dependence of the calculated lattice constant of $\text{Sc}_x\text{Ga}_{1-x}\text{P}$ ternary alloys compared with Vegard's law

Figure 3. Composition dependence of the calculated bulk modulus of $\text{Sc}_x\text{Ga}_{1-x}\text{P}$ ternary alloys compared with the linear concentration dependence prediction.

Figure 2 shows the variation of the lattice constant with increasing composition of x , in which it is compared to the predictions of Vegard's law [24]. We can obviously see that our results are in good agreement with the results obtained by Vegard's law, although there is

very little difference between them which can be explained by the presence of a flexural modulus mainly due to the relaxation of the structure, to the deformation of the crystal.

In addition, in our calculation of the bulk modulus at different compositions of $\text{Sc}_x\text{Ga}_{1-x}\text{P}$ alloys (see Fig. 3), We find a small deviation from the linear dependence in concentration predicted by Vegard's law which can be explained by the same reason we mentioned earlier and is the presence of the bending modulus.

3.2. Electronic properties

3.2.1. Band structures

One of the most important parameters in materials science is the gap energy, because it is directly related to the operating wavelength of electronic components. For example, knowledge of this quantity makes it possible to determine the nature of the material and subsequently the field of their application as an electronic or optoelectronic device. It is therefore possible to widen the field of use of any semiconductor alloy by varying the gap energy according to the composition. Motivated by this reason, we have investigated the electronic properties of the ternary alloys $\text{Sc}_{0.25}\text{Ga}_{0.75}\text{P}$, $\text{Sc}_{0.25}\text{Ga}_{0.75}\text{P}$ and $\text{Sc}_{0.25}\text{Ga}_{0.75}\text{P}$ and taking into account the optimized lattice parameters of each of the alloys considered.

We have determined the gap energies of the binary compounds ScP and GaP whose results are gathered in table. 2. The band structures were calculated according to the directions of high symmetry in the first Brillouin zone of a cubic lattice. To compare our results with the experimental one, the gap energies of the binary compounds were calculated by the approximations (PBE-GGA) [25] and (GGA +TB-mBJ) [26]. It can be noted that (GGA +TB-mBJ) gives better values close to those obtained experimentally.

Semiconductors are characterized by a band gap, which is defined by the distance between the last occupied states of the valence band and the free states of the conduction band. Since the maximum energy of the valence band is at point Γ and the minimum energy of the conduction band at point X, this GaP compound is considered an indirect gap semiconductor. However, the binary compound ScP is a direct gap semiconductor because the maximum of the valence band and the minimum of the conduction band both are located at the same point X.

The figures (4) and (5) shows the band structures of the binary compounds GaP and ScP in zinc-blende phase calculated by the approximations (PBE – GGA) (left panel) and (GGA +TB – mBJ) (right panel).

Figure 4. Band structure of the GaP calculated along high symmetry directions using GGA (left panel) and mBJ (right panel).

Figure 5. Band structure of the ScP calculated along high symmetry directions using GGA (left panel) and mBJ (right panel).

Table 2. Gap energy E_g of $Sc_xGa_{1-x}P$ ternary alloys at equilibrium volume.

E _g (eV)					
System	Present calculation		Other calculations	Experiments	Transition type
	GGA	mBJ			
GaP	1.78*	2.87*	2.80 ^a , 2.80 ^b , 1.81 ^c	2.76 ^j , 2.78 ^h	Direct transition (Γ–Γ)
	1.721*	2.272*	1.44 ^d , 2.24 ^a , 2.32 ^e	2.35 ⁱ , 2.261 ^j	Indirect transition (Γ–X)
Sc _{0.25} Ga _{0.75} P	0.62*	1.91*	1.59 ^e	–	Direct transition (Γ–Γ)
	1.98*	2.81*	–	–	Indirect transition (Γ–X)
Sc _{0.5} Ga _{0.5} P	0.76*	1.39*	1.84 ^e	–	Direct transition (Γ–Γ)
	2.22*	2.67*	–	–	Indirect transition (Γ–X)
Sc _{0.75} Ga _{0.25} P	1.14*	2.04*	0.6 ^c , 1.59 ^e	–	Direct transition (Γ–Γ)
	2.07*	2.47*	–	–	Indirect transition (Γ–X)
ScP	1.291*	1.849*	1.466 ^f	–	Direct transition (X – X)

* Present calculations.

^a Ref [8] using approximation of the virtual crystal with the actual disorder.

^b Ref [27] using approximation of the virtual crystal with the actual disorder.

^c Ref [23] using FP-LMTO + LDA .

^d Ref [21] using FPLAPW + GGA.

^e Ref [21] using the Engel-Vosko (EV) .

^f Ref [28] using FPLAPW + GGA.

^j Ref [29].

^h Ref [30].

ⁱ Ref [2].

The direct $E_{\Gamma \rightarrow \Gamma}$ and indirect $E_{\Gamma \rightarrow X}$ transition energies of the ternary $Sc_xGa_{1-x}P$ alloy were calculated by the approximations (PBE-GGA) and (TB- mBJ). The results obtained from the gap energy are grouped in table (2). Because the maximum of the valence band and the minimum of the conduction band are at the same high symmetry point Γ , therefore the alloys obtained are direct gap semiconductors. The values of the direct and indirect gap energies show a slight shift when the Sc atom moves towards the concentrations 0.25, 0.5 and 0.75. A considerable improvement in gap energy was observed by the approach (TB – mBJ) compared to the approximations (PBE-GGA). These results are considered as theoretical

prediction for this ternary alloy pending experimental confirmation. Figure (5) shows the ternary band structure $\text{Sc}_x\text{Ga}_{1-x}\text{P}$ for concentrations $x = 0.25, 0.50$ and 0.75 , determined by the approximation (TB-mBJ).

Figure 6. Band structures for $\text{Sc}_x\text{Ga}_{1-x}\text{P}$ (8-atom SQS cells) for concentrations of (a) $x = 0.25$, (b) 0.50 , and (c) 0.75 , within the mBJ approximation

3.2.2. Density of states DOS

The density of electronic states quantifies the number of electronic states with a given energy in the material considered. In other words, it represents the number of states available to the electrons. It just depends on the energy. The density of state is an important parameter for the calculation of electronic, optical, chemical and magnetic properties of materials.

The total and partial density of state (DOS) of binary GaP and ScP (zinc-blende) compounds at equilibrium are shown in figure 7. We can distinguish from the origin of the energies, two regions of important valences called VB1 and VB2 and two conduction regions called CB1 and CB2.

In the case of ScP, the first valence region VB1 is composed mainly by the P-3s states, the second valence region VB2 is dominated by the Sc-3d and P-3p states. The Sc-3d state essentially participates in the first conduction region CB1. The second CB2 conduction region is dominated by the 3d and 3p states for the Sc and P atoms, respectively.

For GaP compound, P-3s state contributes to the first valence region VB1, while the second valence region VB2 is dominated by Ga-4s and P-3p states. The first conduction region CB1 is dominated by the mixed contribution of Ga-4s, Ga-4p, P-3s and P-3p states; however, the second conduction region CB2 is dominated by the Ga-4p and P-3p states.

The total density of state of the ternary alloys $\text{Sc}_{0.25}\text{Ga}_{0.75}\text{P}$, $\text{Sc}_{0.5}\text{Ga}_{0.5}\text{P}$ and $\text{Sc}_{0.75}\text{Ga}_{0.25}\text{P}$ are shown in Figure (8). We can distinguish with four distinct regions, two regions of VB1, VB2 valences and two other regions of conduction bands CB1 and CB2, which are separated by the gap energy E_g . The first valence region VB1 is dominated by P-3s states with a small contribution from Ga-4p and P-3p states, the second valence region VB2 is essentially composed of Ga-4p and P-3p states. The first conduction band CB1 is dominated by Sc-3d, Ga-4p and P-3p states while the Ga-4p and P-3p states contribute to the second conduction region CB2.

3.3 Optical Properties

Semiconductor physics is concerned with the study of the optical properties of materials due to their major roles in electronic and optoelectronic component technology. Optical properties occur during the interaction between an electromagnetic wave and matter, i.e. when the semiconductor is subjected to an external disturbance such as light. Many optical phenomena occur when light radiation passes through the material, such as absorption, reflection, refraction, scattering, transmission and emission. To better understand these phenomena, one must study the dielectric function in the framework of quantum

mechanics, then we have to see the link between the real and imaginary parts of the dielectric function, as well as the complex index through the Kramers-Kronig equations [33]. The dielectric function is written as:

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i \varepsilon_2(\omega) \quad (1)$$

Figure 7. Calculated total density of states (DOS) of binary compounds ScP and GaP

Figure 8. Calculated total density of states (DOS) of $\text{Sc}_x\text{Ga}_{1-x}\text{P}$ alloys

Where the imaginary part $\varepsilon_2(\omega)$ of this dielectric function depends on the frequency and is directly related to the band electronic structure and can be determined by summing all possible transitions from occupied states to empty states using the following expression [34]:

$$\varepsilon_2^{ij} = \frac{4\pi^2 \varepsilon^2}{\Omega m^2 \omega^2} \sum_{knn'\sigma} \langle kn\sigma | p_i | kn'\sigma \rangle \langle kn'\sigma | p_j | kn\sigma \rangle f_{kn} (1 - f_{kn'}) \delta(e_{kn} - e_{kn'} - \hbar\omega) \quad (2)$$

f_{kn} is the Fermi-Dirac distribution function, $|kn\sigma\rangle$ is the wave function of the considered crystal, corresponding to the same eigenvalue of k and σ (spin). The summation is made on all the states of the Brillouin irreducible zone.

The real part $\varepsilon_1(\omega)$ is derived from the imaginary part of the dielectric function by the Kramers - Kronig transformation according to the following relation [33]:

$$\varepsilon_1(\omega) = 1 + \frac{2}{\pi} P \int_0^\infty \frac{\varepsilon_2(\omega') \omega' d\omega'}{\omega'^2 - \omega^2} \quad (3)$$

where ω is the frequency, P is the main part of the Cauchy integral.

Another important complex quantity related to the dielectric function is used to describe the medium, it is the refractive index, which is given by the relation [35], [36]:

$$n(\omega) = \left[\frac{\varepsilon_1(\omega)}{2} + \frac{\sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)}}{2} \right]^{1/2} \quad (4)$$

When the frequency cancels ($\omega = 0$), equation (4) is simplified by :

$$n(0) = \varepsilon^{1/2}(0) \quad (5)$$

The extinction coefficient $K(\omega)$ is given by the following relationship [35], [36]:

$$K(\omega) = \frac{1}{\sqrt{2}} [(\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega))^{1/2} - \varepsilon_1(\omega)]^{1/2} \quad (6)$$

Figure (9.a) shows the variation of the real part as a function of energy for the ternary alloy $\text{Sc}_{0.5}\text{Ga}_{0.5}\text{P}$. The main characteristics of this curve are as follows: with a peak at about 2.275 eV, the spectrum of the real part decreases with increasing photon energy in the region bounded by (2.275, 3.674 eV). The optical dielectric constant $\varepsilon_1(0)$ calculated at normal pressure has the value $\varepsilon_1(0) = 11.483$.

Figure (9.b) of the absorption spectrum with the generalized gradient approximation parameterized of Perdew-Burke-Ernzerhof (PBE-GGA) shows that the threshold energy (the fundamental transition) of the dielectric function is about 1.443 eV. This value represents the direct optical transition from the top of the VB to the bottom of the CB according to the point Γ . The Point A representing the direct transition to Γ followed by three fundamental peaks: (i) the peak (B) located at 2.851 eV first absorption for electron transitions from the R point of the valence band to the R point of the conduction band, (ii) the peak (C) located at 5.02 eV represents the $X_V - X_C$ transitions, (iii) the peak (D) located at 5.54 eV represents the MV-Mc transitions.

The refractive index is also calculated for the ternary alloy $\text{Sc}_{0.5}\text{Ga}_{0.5}\text{P}$, the results are shown in figure (9.c), the three major peaks were located at energies 1.924 eV, 2.158 eV and 2.519 eV relative to the magnitudes $n = 4.535$, 4.495 and 4.442. After the third main peak the spectrum of $n(\omega)$ decreases dramatically with increasing photon energy.

The refraction phenomenon disappears since the refractive index becomes almost equal to 0.5, and the material behaves like a free space. From this minimum, the variation of the

refractive index is small and therefore the dispersion is very low. It can be noted that the dispersion phenomenon is very important in the region of the visible spectrum. This large variation in refractive index in the visible region of the spectrum does not allow the material to be used in the manufacture of optical fibers.

The evolution of the extinction coefficient K is shown in figure (9.d).the extinction or attenuation coefficient represents the absorption phenomenon in the complex refractive index and is directly related to the absorption coefficient, so that the extinction coefficient only starts to increase from a threshold, which represents the optical gap. This threshold is equal to 1.224 eV and it starts to increase to reach a maximum at an energy of 3.551 eV.

These results which we obtained for the optical constants are considered as the first published for the ternary alloy $\text{Sc}_{0.5}\text{Ga}_{0.5}\text{P}$, because no theoretical or experimental study was found.

Figure 9. The calculated (a) $\epsilon_1(\omega)$ real, (b) $\epsilon_2(\omega)$ imaginary parts of complex dielectric constant, (c) the refractive index $n(x)$ and (d) the extinction coefficient $K(x)$ of $\text{Sc}_{0.5}\text{Ga}_{0.5}\text{P}$ ternary alloys.

4. Conclusion

In this summary, we have studied the structural, electronic and optical properties of ternary alloy $\text{Sc}_x\text{Ga}_{1-x}\text{P}$ with their constituents ScP and GaP, which crystallize in NaCl and zinc-blende (ZnS) phases, respectively.

Our calculations were performed using the *ab-initio* Full-Potential Linearized Augmented Plane Waves (FP-LAPW) method.

The first main step of this work is devoted to the determination of the structural properties at equilibrium where the lattice parameter, the bulk modulus and its derivative with respect to pressure were obtained from the equation of state of Murnaghan. The results obtained show that the lattice parameter of the cubic ternary alloy $\text{Sc}_x\text{Ga}_{1-x}\text{P}$ increases with the increase in the composition x , therefore there is a perfect agreement between Vegard's law and the formalism of the functional density theory (DFT) has been established, while the bulk modulus of this alloy shows a small deviation from linearity. We have compared these results with other theoretical and experimental studies available in the literature.

The second part of this work is dedicated to the calculation of the electronic properties, indeed we have determined the band structure and the electronic density of state (DOS) of the considered materials. The most important result obtained in this case is the gap energies calculated by the Tran-Blaha modified Beck-Johnson potential (TB-mBJ), for which the gap value for each semiconductor material is significantly improved compared to the experimental results.

All the ternary alloys formed from those binary compounds exhibit a direct transition ($\Gamma \rightarrow \Gamma$) according to the high symmetry point Γ .

Finally, we have calculated the optical properties of the resulting semiconductors. The dielectric function and refractive index are determined, our results obtained for the optical constants are considered as the first published for the ternary alloy $\text{Sc}_{0.5}\text{Ga}_{0.5}\text{P}$.

Acknowledgements

The authors thank the Laboratory of Micro and Nanophysics (LaMiN), National Polytechnic School Oran, ENPO-MA Oran, Algeria and Magnetic Materials Laboratory, Faculty of Exact Sciences, Djillali Liabes University of Sidi Bel-Abbes, Algeria and the Ministry of Higher Education and Scientific Research of Algeria for their supported during the development of this work.

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