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First-principles study of fundamental properties of BX (X= As, P,N and Bi) compounds

***Yousra Megdoud*[1,2], *Yamina Benkrima*[3], *Latifa Tairi*[4], *Redha Meneceur*[5], *Sebti Ghemid*[2], *Hocine Meradji*[2]**

[1]Institute of Sciences, Centre University Morsli Abdallah Tipaza, Algeria
[2]LPR Laboratory, Départment of Physics, Faculty of Science, Badji Mokhtar University, Annaba, Algeria
[3]Ecole Normale Supérieure de Ouargla, 30000 Ouargla, Algeria
[4]Research Center in Industrial Technologies CRTI, P.O. Box 64, Cheraga16014 Algiers Algeria
[5]Unit for the Development of Renewable Energies in Arid Zones (UDERZA), El Oued University, Algeria

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Ab initio calculations were carried out on the structural, electronic, thermal and optical properties of the binary compounds BP, BAs, BN and BP in the different phases: zinc blende (B3), NaCl (B1), CsCl (B2), NiAs (B8) and wurtzite (B4).We used the augmented linearized plane wave method (FP-LAPW) based on the density functional theory (DFT). The exchange-correlation potential (XC) was processed through the generalized gradient approximation developed by Wu-Cohen (WC-GGA) to optimize the appropriate structural parameters. Moreover, the modified Becke-Johnson (mBJ) method is used to determine the electronic band structure of BP, BAs, BN and BBi semiconductors. Optical properties were studied: dielectric function, refractive index, absorption coefficient and reflectivity.The results assert that the zinc blende structure is the stable phase with an indirect band gap.

Keywords: Density functional theory DFT, FPLAPW method, mBj, band-gap, optical properties and Wc-GGA

Першопринципне дослідження фундаментальних властивостей сполук BX (X= As, P,N і Bi). *Yousra Megdoud, Yamina Benkrima, Latifa Tairi, Redha Meneceur, Sebti Ghemid, Hocine Meradji*

Ab initio розрахунки були проведені щодо структурних, електронних, термічних та оптичних властивостей бінарних сполук BP, BAs, BN та BP у різних фазах цинкової обманки (B3), NaCl (B1), CsCl (B2), NiAs (B8) і вюрцита (B4). Ми використовували розширений метод лінеаризованої плоскої хвилі (FP-LAPW), заснований на функціональній теорії щільності (DFT). Обмінно-кореляційний потенціал (XC) був оброблений за допомогою узагальненої градієнтної апроксимації, розробленої Wu-Cohen (WC-GGA), щоб оптимізувати відповідні структурні параметри. Крім того, модифікований метод Беке-Джонсона (mBJ) застосовано для визначення електронної зонної структури напівпровідників BP, BAs, BN і BBi. Досліджено оптичні властивості: діелектричну функцію, показник заломлення, коефіцієнт поглинання та відбивну здатність. Результати стверджують, що структура цинкової обманки є стабільною фазою з непрямою забороненою зоною.

1. Introduction

The behavior of metals, alloys and compounds under high pressures is of great current interest because high pressure experiments are becoming more refined [1-2]. Therefore, an accurate first-principles method of calculating the structural properties of all these matters is very valuable. Such calculations can also predict pressure-induced phase transitions. Theoretical studies of such phase transitions in compounds have attracted particular interest in the last three decades [3-5]. Among the various compounds, boron compounds are of great interest, namely BP, BAs, BN and BBi; under normal conditions they have a zinc blende (ZBC) structure and are the subject of numerous experimental and theoretical studies [6-11]. The boron compounds are expected to find application in optoelectronic devices due to some extreme physical properties, such as low ionicity, small band gap, short bond lengths and high mechanical strength or elastic moduli, as well as high melting point [6-9]. Theoretical work on boron compounds has so far been widely carried out, mainly by Ferhat et al. [8, 12-14] through various *ab initio* methods. Recently, the structural and electronic properties of BX compounds have been calculated by Ferhat et al [12-16], Zaoui et al [15], Carrier et al [17], and Meradji et al [18] using the various first-principles methods based on the density functional theory (DFT). They reported that the zinc-blende (ZB) phase (B3) is the ground state of BSb, BSb and BP. The most recent work on these alloys is done by K. Boumama et al. [19]. They theoretically predicted the phonons of these alloys and confirmed the experimental work by Sanjurjo et al. [20].

This paper is organized as follows: 'Section 2 describes the BP, BAs, BN and BBi binary compounds using wien2K code based on the density functional theory DFT; confirmation of the results obtained based on it on materials used in optoelectronics is given in Section 3. Finally, Section 4 summarizes the conclusions of the paper and lists the corresponding references.

2. Computational details

All the calculations presented in this work were carried out by the plane wave method linear Augmented (FP-LAPW) within the framework of Density Functional Theory (DFT) [21-23] using Wien2K code [24]. For structural properties, the correlation exchange potential was calculated by the generalized gradient approximation (GGA) in the new form (WC-GGA) proposed by Wu and Cohen (WC-GGA) [25]. The recent approximation proposed by Becke and Johnson (mBJ: modified Becke-Johnson) [26] was also used to study band structures. In the FP-LAPW method, the space is divided into non-overlapping 'muffin-tin' (MT) spheres around atomic sites and an interstitial region (IR). Inside the MT spheres, the basis sets are described by radial solutions of the one-particle Schrödinger equation and their energy derivatives multiplied by spherical harmonics. In the interstitial region, the basic set consists of plane waves. However, in the calculations presented here, the plane wave cutoff with the condition RMT*$K_{\max} = 8$ was used, where RMT is the smallest radius of a muffin-tin sphere and $K_{\max}$ is the largest vector k in the plane wave expansion. Accordingly, the muffin-tin radii for the four atoms were taken as R_{MT}(B)=1.6, R_{MT} (Bi) = 2.46, R_{MT} (P) = 2.2, R_{MT} (As) = 2.05 and R_{MT} (N) = 2.0 a.u. The maximum value of the expansion of the wave function inside the atomic spheres was limited to $l_{\max} = 10$. The charge density was extended to up to $G_{\max}$ = 14 (Ryd) 1/2. A mesh of 47 special k-points for binary compounds and 36 k-points for ternary alloys was taken from the irreducible region of the Brillouin zone. Self-consistent calculations are considered to be converged when the total energy is stable at 0.1 mRy.

3. Results and discussion

3.1. Structural Properties

The structural characteristics of BP, BAs, BN and BBi compounds were determined through an energy minimization process using the (WC-GGA) method; for others to optimize the volume, the total energy was calculated as a function of the unit cell volume using the c/a experimental ratio. The lattice parameters corresponding to the minimum energy were estimated using this approach. The unit cell energy was plotted against the volume and fitted using the Birch-Murnaghan equation of state [27]:

$$E(V) = \\ = \frac{B_0 V}{B_0'}\left[\frac{(V_0/V)^{B_0'}}{B_0'-1} - 1\right] + E(V_0) - \frac{B_0 V}{B_0'-1} \cdot \quad (1)$$

Here E, V_0, B and B' are respectively: the total energy, the equilibrium volume, the compress-

Table 1 : The lattice parameters (in Å), the c/a ratio, the internal parameter (in Å), the compressibility modulus (in GPa), its pressure derivative and its equilibrium energy E0 (in Ry) of the different phases considered for compound BP.

BP	a	c	c/a	B	B’	E0
RS (B1) This work WC-GGA	4.3069			169.5037	3.9588	733.2159
LDA PBE-GGA Experiment Calculation	4.2729			177.7375	4.0579	-731.1849
	4.3276			161.9762	4.2345	-733.8020
	4.327a			155a2.9800a		
	4.320b			171b2.82b		
	4.339c			155c		
	4.332d			161d		
	4.32j			156.822j		
ZB (B3) This work WC-GGA LDA PBE-GGA Experiment Calculation	4.5250			169.1176	3.7726	- 733.366
	4.4946			175.6060	3.7709	- 731.3366
	4.5523			161.3763	3.7916	- 733.9602
	4.538e,f , g173e, f, g					
	4.558d			166d 4d		
	4.546h			166h	3 h	
CsCl (B1) This work WC-GGA	2.7083			141.7342	3.8937	-733.1026
LDA PBE-GGA Experiment Calculation	2.6865				3.1755	-731.0687
	2.7238			143.5897	3.3451	-733.6883
				133.5993		
NiAs (B8) This work WC-GGA LDA PBE-GGA Experiment Calculation	3.1993	5.2281	1.6341	169.5081	3.7858	- 1466.7305
	3.1420	5.2157	1.6600	170.9170	3.9570	- 1468.2217
	3.2168	5.3080	1.6501	165.2083	3.8933	- 1450.7702
Wurtzite This work WC-GGA (B4) LDA PBE-GGA Experiment Calculation	3.0492	5.0879	1.6686	158.8082	5.2567	- 1466.3946
	3.0268	5.0326	1.6627	162.1720	6.0124	- 1497.2010
	3.1055	5.1389	1.6548	159.7136	5.2467	- 1459.1236

aRef [30], bRef [56], cRef [13], dRef [39], eRef [57], fRef [16], gRef [17], hRef [18], iRef [58], jRef [59].

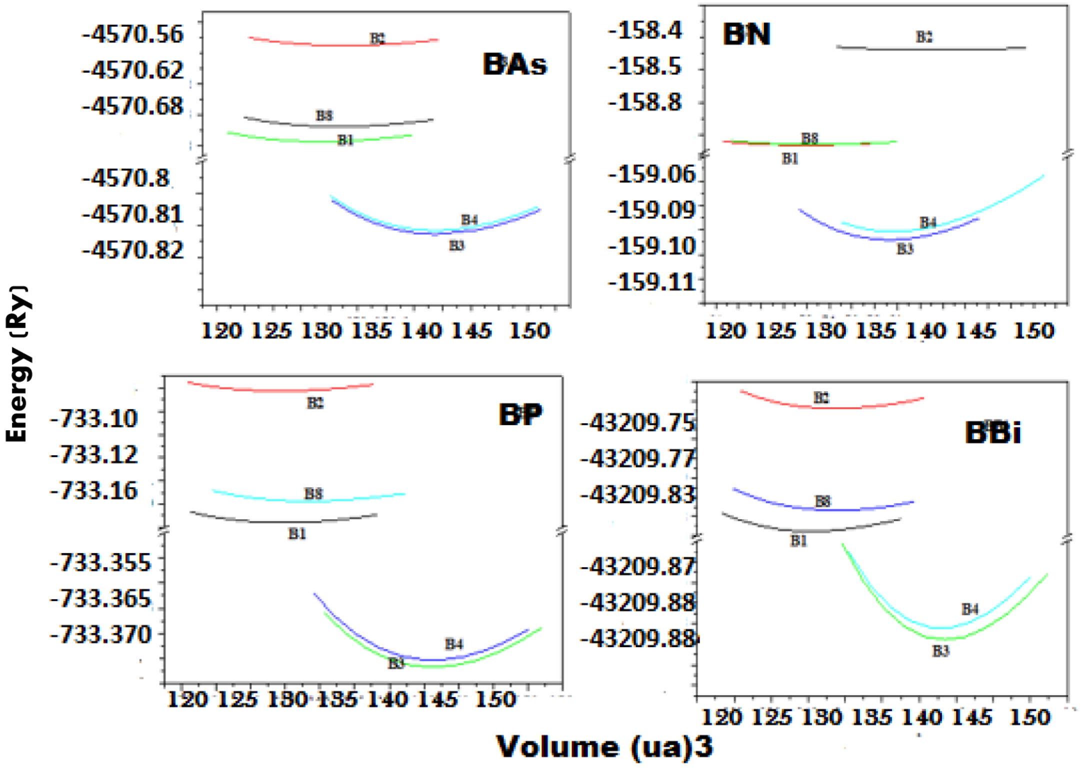

Fig. 1. Total energy versus volume calculated in zinc blende (B3), NaCl (B1), CsCl (B2), NiAs (B8) and wurtzite (B4) phases for compounds BBi. BAs, BN and BP.

ibility modulus and its derivative. The compressibility modulus is given by:

$$B_0 = V\frac{\partial^2 E}{\partial V^2} \qquad (2)$$

3.1.1 Phase stability

First, we calculate the phase stability of the binary compounds BAs, BBi, BN and BP. The phases considered in this study are: zinc blende ZB (B3), NaCl (B1), CsCl (B2), wurtzite WZ (B4) and NiAs (B8). To achieve this, we calculate the total energy as a function of volume for each compound in the different phases; the curves obtained are fitted to the Murnaghan equation [27]. The results are given in Fig (1). According to these curves, it can be seen that the zinc blende phase is the most stable phase, which is explained by the occupation of the lowest energy level. This result is consistent with that of Ustundag et al. [28] using the FP-LAPW method. As seen from these curves, the difference between the minimum energy values of the wurtzite phase (B4) and the zinc blende phase (B3) is very small. The same case is observed for the NiAs (B8) and NaCl (B1) structures. We can explain this behavior by the binding mechanism in these structures, namely coordination.

NaCl and NiAs have six-fold coordinate structures, while wurtzite and zinc-blende structures are quadruple. This similarity in chemical bonding leads to similar fundamental energies. However, the CsCl phase has a higher energy than the other phases, which means that this structure is unstable under ambient conditions but can be obtained at higher pressures. The calculated structural parameters such as the lattice constants (*a* and *c*), the *c*/*a* ratio, the compressibility modulus (*B*), its pressure derivative (*B'*) and its energy at equilibrium (E_0) for the structures considered, as well as the experimental and theoretical data available for the compounds studied and wurtzite are given in Tables (1-2); for the others, the values obtained are predictions and can serve as a reference for future work on these materials. A reasonable agreement is found between our calculated structural parameters and those given in the literature.

2.2.2 Phase transition

Under given conditions of temperature, pressure and composition, we define the phase as the homogeneous part of a crystal system having a known atomic arrangement. When pressure is applied, the distance between the atoms is changed, leading to a new phase. In fact, the pressure affects the chemical bonds and therefore changes the physical properties

Table 2. Lattice parameters (in Å), the c/a ratio, the internal parameter (in Å), the compressibility modulus (in GPa), its pressure derivative and its equilibrium energy E_0 (in Ry) of the various phases considered for the BAs compound.

BAs		a	c	c/a	B	B'	E_0
RS (B1)	This work WC-GGA	4.5905			135.0548	3.6802	-4570.6757
	LDA	4.5502			146.2145	4.1851	-4565.2683
	PBE-GGA	4.6258			124.4247	3.7659	-4571.7650
	Experiment						
	Calculation						
		4.619^a			135^a	3.44^a	
		4.583^b			143^b		
ZB (B3)	*This work WC-GGA*	4.7765			140.0776	4.0496	-4570.8027
	LDA	4.8148			131.3025	3.9698	-4571.8985
	PBE-GGA	4.8135			130.7531	4.3923	-4571.8984
	Experiment						
	Calculation						
		4.777^c					
		$4.77^{d,e}$			$145^{d,e}$		
		4.726^f			147^f	3^f	
		$4.784^{g,h}$			$145^{g,h}$	$3^{g,h}$	
CsCl (B1)	*This work WC-GGA*	2.9170			114.9917	4.3663	-4570.582
	LDA	2.8891			123.1169	4.3719	-4565.1700
	PBE-GGA	2.9409			105.1903	4.7145	-4571.6717
	Experiment						
	Calculation						
NiAs (B8)	*This work WC-GGA*	3.2536	5.3796	1.6534	134.0138	4.1652	-9141.3223
	LDA	3.2212	5.3474	1.6602	129.3689	3.9965	-9132.8964
	PBE-GGA	3.2469	5.3534	1.6488	132.3210	4.0369	-9131.8974
	Experiment						
	Calculation						
Wurtzite (B4)	*This work WC-GGA*	3.3236	5.4740	1.6436	140.1808	4.0894	-9141.6031
	LDA	3.3036	5.4493	1.6698	138.2215	3.9871	-9141.36985
	PBE-GGA	3.3130	5.4952	1.6587	139.9987	4.0033	-9141.5994
	Experiment						
	Calculation						

^{a}Ref [56], ^{b}Ref [18], ^{c}Ref [39], ^{d}Ref [30], ^{e}Ref [57], ^{f}Ref [60], ^{g}Ref [58], ^{h}Ref [59].

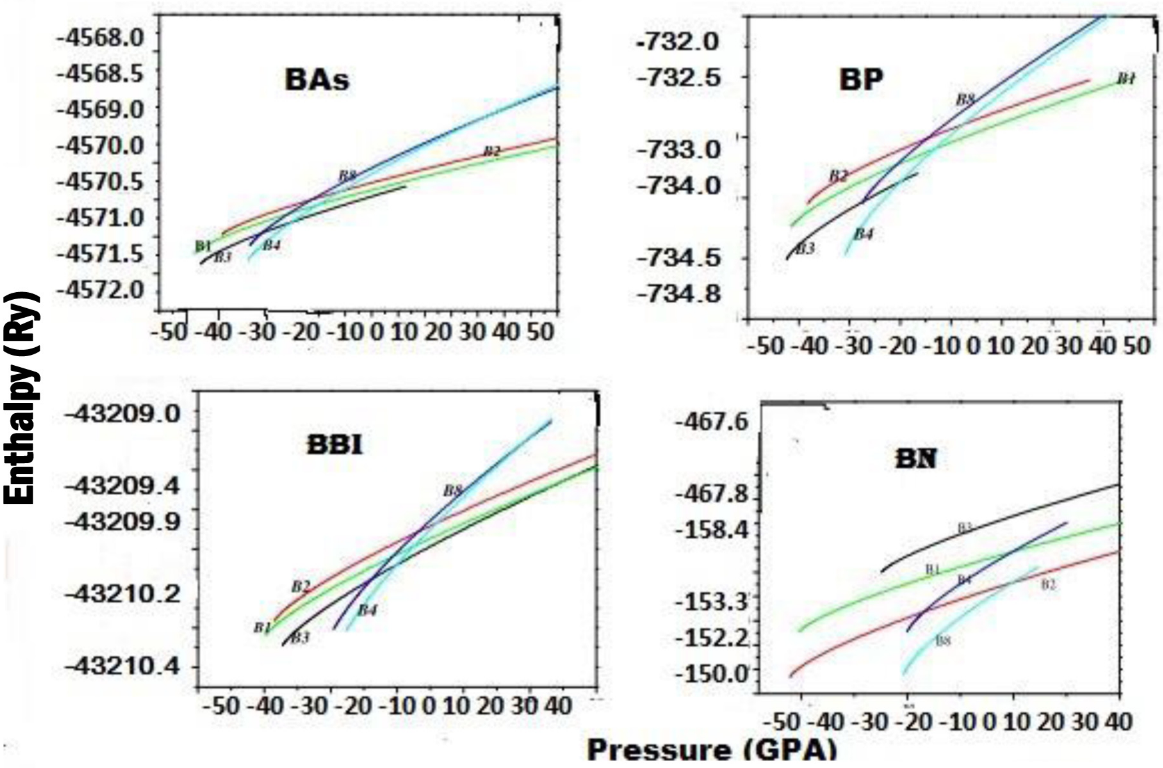

Fig.2: Change in enthalpy as a function of the pressure of the compounds BP, BAs, BBi and BN in the phases of zinc blende (B3), NaCl (B1), CsCl (B2), NiAs (B8) and wurtzite (B4).

Table 5: Calculated transition pressures for the studied binary compounds.

Pt (GPa)		
	Present work	Other calculates
BP		
$B_3 \rightarrow B_1$	130.66	118a, 110b, 160c, 111d
$B_3 \rightarrow B_2$	183.94	
$B_3 \rightarrow B_8$	199.74	
$B \rightarrow B_4$	137.96	
BAs		
$B_3 \rightarrow B_1$	97.89	98a, 93b, 110e, 141f, 105g, 125h(exp)
$B_3 \rightarrow B_2$	209.79	
$B_3 \rightarrow B_8$	142.11	
$B_4 \rightarrow B_1$	98.64	
$B_4 \rightarrow B_8$	154.72	
$B \rightarrow B_2$	232.10	
BBi		
$B_3 \rightarrow B_1$	23.86	
$B_3 \rightarrow B_2$	43.98	
$B_3 \rightarrow B_8$	65.54	
BN		
$B_1 \rightarrow B_4$	0.7587	
$B_1 \rightarrow B_8$	38.1661	
$B_3 \rightarrow B_8$	51.0971	

[a]Ref [12], [b]Ref [31], [c]Ref [79], [d]Ref [80], [f]Ref[81], [g]Ref [82], [h]Ref [32]

Table 6. Bandgap energy E_g (eV) for binary compounds BBi, BAs, BP and BN using the WC-GGA approximation, mBJ

Eg	Our calculations		Exp	Other calculations
	WC-GGA	mBj		
BP				
Zinc blende “ $\rightarrow \Delta_{min}$	1.103	1.8190	-	1.24b,d(GGA), 1.91b(mBj), 1.831g, 1.87h, 1.85k(mBJ), 1.147k(WC-GGA), 1.863l(mBj)
Wurtzite “ $\rightarrow M$	1.542	2.3162		
NaCl	Metallic	Metallic		
CsCl	Metallic	Metallic		
NiAs	Metallic	Metallic		
BAs				
Zinc blende “ $\rightarrow$ ”$_{min}$	1.163	1.690	1.60e	1.21d(GGA), 1.25f, 1.821g(mBj), 1,93e, 1.674i, 1.686m(mBJ) , 1.092m
Wurtzite “ $\rightarrow M$	1.321	2.033		
NaCl	Metallic	Metallic		
CsCl	Metallic	Metallic		
NiAs	Metallic	Metallic		
BBi				
Zinc blende	Metallic	Metallic		0.35a, 0.949b and Metallic c
Wurtzite	Metallic	Metallic		
NaCl	Metallic	Metallic		
CsCl	Metallic	Metallic		
NiAs	Metallic	Metallic		
BN				
Zinc blende “ $\rightarrow$ ”$_{min}$	4.479	5.6131	6.3j	6.31k , 4.19l, 4.40m, 4.38n
Wurtzite “ $\rightarrow K$	5.844	6.0432		5.81P
NaCl “ $\rightarrow K$	5.986	6.679		
CsCl	Metallic	Metallic		
NiAs	Metallic	Metallic		

[a]Ref [90], [b]Ref [91], [c]Ref [37], [d]Ref [14], [e]Ref[92], [f]Ref[18,39], [g]Ref [60], [h]Ref [93] , [i]Ref [94], [j]Ref [38], [k]Ref [92], [l]Ref[95], [m]Ref[40], [n]Ref [45],[p]Ref [44].

of the material. The transition pressure from one phase to another is determined using the Gibbs free energy which is given by the following relationship:

$$G = E + HP + ST \quad (3)$$

Since we performed our calculations for the temperature $T = 0$, in this case the Gibbs energy is reduced to the enthalpy H = E + PV. By plotting enthalpy against pressure for each structure, the transition pressure is obtained when the enthalpies of the structures under consideration are equal. In the Fig. 5, we present the enthalpies calculated as a function of the pressure for the different structures of BAs and BPs. The calculated phase transition pressures between the considered phases are given in Table 5 along with the previous theoretical and experimental results. From this table it follows that for the BP compound, the calculated pressure of transition from the zinc blende phase (B3) to that of NaCl (B1) reasonably cor-

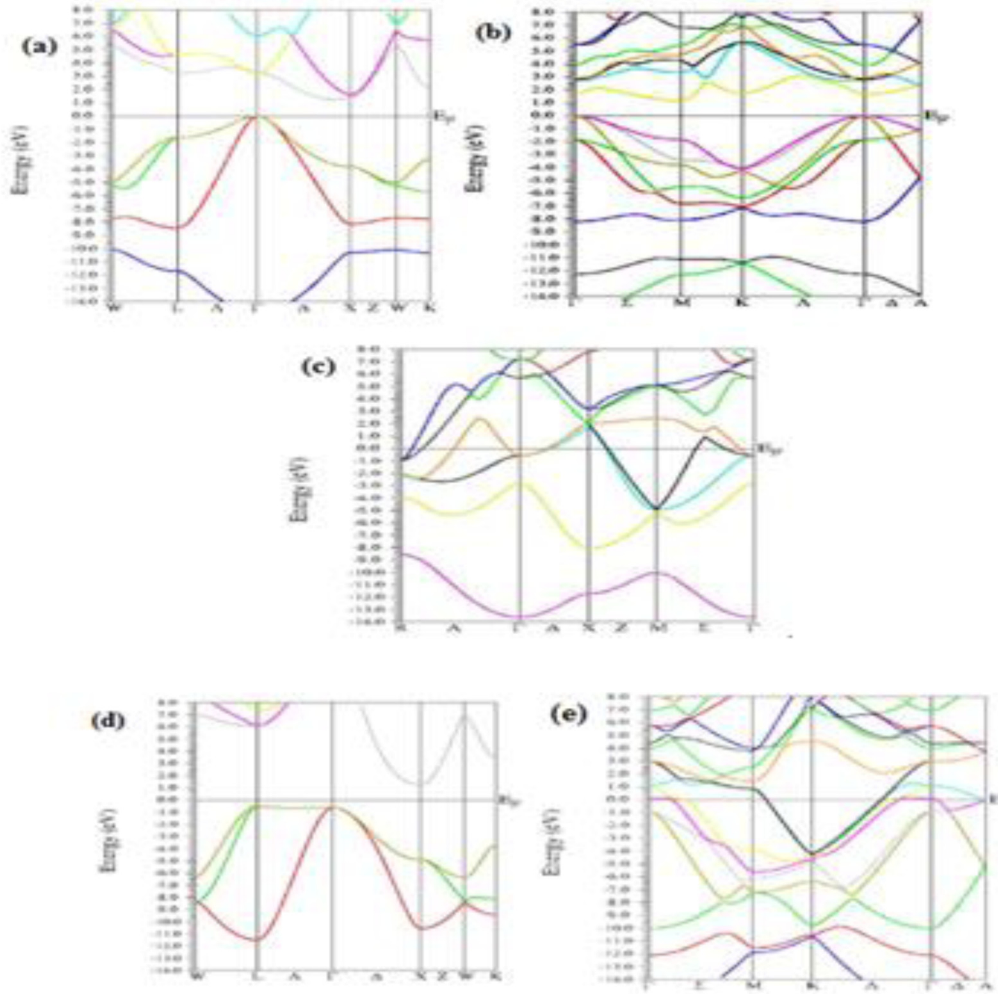

Fig 3. Band structure of (a) BP (zinc blende/WC-GGA), (b) BAs (wurtzite/WC-GGA), (c) BBi (CsCl/WC-GGA), (d) BN (NaCl/mBj) and (e) BP (NiAs/mBj).

responds to the theoretical results. For the BAs compound, the phase transition is between the phases mentioned above; the calculated transition pressure value is in good agreement with those reported by Thakore et al. [29], Sarwan et al. [30] and Mehl et al. [31]. As can be seen, the value we obtained is lower than the experimental one [32]. The other results are predictions and can serve as a reference for future work on these compounds.

3.2 Electronic Properties

In solid-state physics, band theory is a quantum model giving the possible energies of electrons in a solid. It explains the electrical behavior of different materials between an insulator, a semiconductor and a conductor. The compounds under study are identified as semiconductors important for their efficient use in light-emitting diodes (LEDs) and photovoltaic designs [33-35]. Their energy bands are calculated along important symmetry directions in the Brillouin zone for the studied phases using both WC-GGA and mBJ approximations. Guided by this reason, we began to study the electronic properties of the binary compounds BBi, BAs, BN and BP.

The band structures were calculated according to the directions of high symmetry in the first Brillouin zone of cubic and hexagonal lattices (zinc blende, NaCl, CsCl, NiAs and wurtzite); they are illustrated in Fig 3. These compounds are semiconductors with band gaps (Γ-Δ_min) and (Γ-M) in zinc blende and wurtzite structures, respectively. Δ_min is a point located along the high symmetry direction Δ. In the other structures studied, the compounds exhibit metallic behavior that is related to the bonding mechanism in these structures. Direct bandgap structures have excellent optical properties and can be used as light detectors or light emitters. (LEDs, lasers) **[33-35]**. Indirect gap structures cannot interact with light without heat. This greatly disturbs their electronic properties and lead to electron-phonon type interactions with very poor light emission. The numerous bandgap values are given in Table 5. From this table, it can be noted that for the zinc blende compounds, the band gap calculated in mBJ is consistent with the theoretical values in the same approximation and is quite close to the experimental values [36, 37]. In the BAs compound, the band gap obtained using WC-GGA is closer to the theoretical value for the reference [38, 18, 40]. In mBJ calculation, the band gap is slightly higher than the experimental one and matches that obtained by Benchehima et al. [40]. It is well known that the mBJ approach gives energy band gaps in good agreement with experiments [41].

3.3. Optical Properties

The physics of semiconductors consists in studying, among other things, the optical properties of materials with a view to their primordial roles in the technology of electronic and optoelectronic components. The optical properties are associated with the interaction between the electromagnetic wave and the matter, when the semiconductor is subjected to an external irradiation such as light. Many optical phenomena take place when the material is irradiated by light, such as absorption, reflection, refraction, diffusion, transmission and emission. To better understand these phenomena, we will study the dielectric function in the context of quantum mechanics to see the existing relationship between the real and imaginary part of the dielectric function, as well as the complex index, through the Kramers-Kronig equations.

The dielectric function is written in the form $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$; it makes it possible to describe the optical properties of the media for all photons of energy E=??ω. The frequency dependent imaginary part $\varepsilon_2(\omega)$ of this dielectric function is directly related to the electronic band structure and can be determined by summing all possible transitions from occupied to empty states using the following expression [42]:

$$\varepsilon_2(\omega) = \\ = \frac{4\pi^2 e^2}{m^2\omega^2}\sum_{i,j}|i|\,M|\,j|*f_i(1-f_i(\omega)-h\omega)d^3k \quad (4)$$

The summation is carried out over the first Brillouin zone, and the elements of the dipole moment are given by $rM_{cv}(k) = u_{ck}|\,e\nabla|\,u_{vk}$, from where e is a potential vector which expresses the electric field. The matrix element $M_{cv}(k)$ is a product that represents the direct transition between the valence band states u_{vk}(r) and the conduction band states $u_{ck}(r)$. The energy term $\hbar\omega_{cv}(k) = E_{ck} - E_{vk}$ is the energy corresponding to this transition. 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 relationship:

$$\varepsilon_1(\omega) = 1 + \frac{2}{\pi}P\int_0^\infty \frac{\varepsilon_2(\omega')\omega' d\omega'}{\omega'^2 - \omega^2}\ , \quad (5)$$

where ω is the frequency, P is the principal part of the Chauchy integral.

To describe the medium, another important complex quantity associated with the dielectric function is used – the refractive index, which is determined by the relation:

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

The knowledge of the real part and the imaginary part of the dielectric function is important, so that one can determine the index of refraction. Other theoretical and empirical models are widely used to estimate the refractive index; in this study, we will focus on the following models:

The expression proposed by Ravindra et al [43]:

$$n = \alpha + \beta E_g$$

With, α = 4.084 and β= 0.62

The empirical relationship of Herve and Vandamme [44]:

$$n = \sqrt{1 + \left(\frac{A}{E_g + B}\right)^2}$$

With, A= 13.6 eV and B= 3.4 eV

The absorption coefficient α(ω) corresponds to the energy emitted per unit time, volume, and divided by the energy flux. It is defined by the following equation:

$$\alpha(\omega) = \frac{4\pi}{\lambda}k(\omega) \quad (7)$$

$\alpha(\omega)$ is linked to ε_2 by the relation:

$$\pm(\ddot{\text{Й}}) = \frac{{}_2()}{\text{n}(\ )\text{c}} \quad (8)$$

In the calculations of optical properties of the binary compounds BX(X=N, As, Bi, and P) by the WC-GGA approximation, we used the

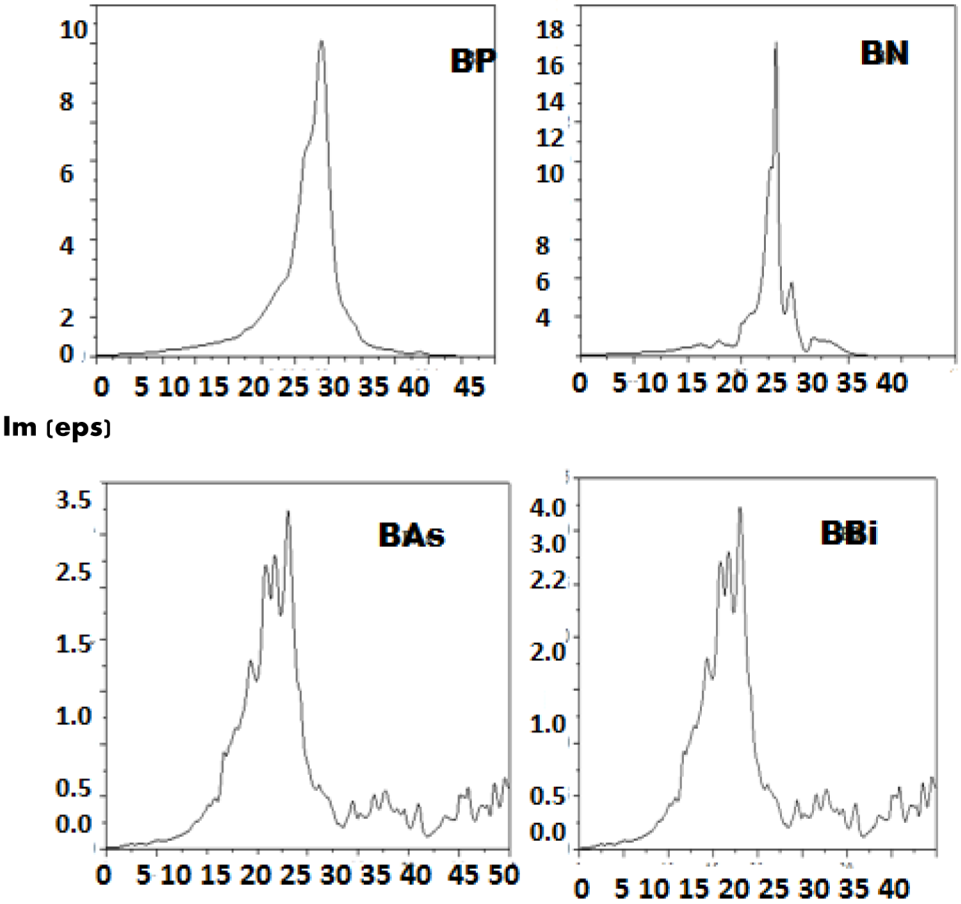

Fig.4. Variation of the imaginary part of the dielectric function depending on energy for compounds BP, BN, BAs and BBi.

equilibrium lattice parameter and a number of 3000 points k in the Brillouin zone (3 times the value of k points in the calculations of the structural properties, which require great accuracy), since the calculation of these properties requires a large number of eigenvalues corresponding to eigenvectors.

Figs. 4 and 5 represent real and imaginary parts of the dielectric function depending on the energy of the binary compounds BP, BN, BBi and BAs. We note that the imaginary part has a major peak between two other small bumps. The major peaks of the binary compounds BP, BN, BBi and BAs are located at the energies 21.9655 eV, 28.2643 eV, 18.0313 eV and 20.7183 eV, respectively, with a noticeable deviation in their amplitudes towards higher energies; these results are illustrated in the Fig 5. Subsequently, the first critical points (right) occur at 5.9153 eV, 11.3822 eV, 1.2241 eV and 5.3065 eV for the BP, BN, BBi and BAs respectively. The first critical points correspond to the direct optical transition between the top of the valence band and the bottom of the conduction band at point Γ.

According to the Fig 5, the spectra of the real part of the dielectric function increase with an increase in photon energy outside the regions delimited by (4.9320, 6.1916 eV), (9.1105, 12.2885 eV), (1.4456, 4.3589 eV) and (3.2658, 5.7198 eV) for compounds BP, BN, BBi and BAs, respectively. On the other hand, inside the same previous regions, the real parts decrease with increasing photon energy. The first region corresponds to normal dispersion, while the second region is said to be abnormal dispersion. We also notice that the spectra of the dielectric function have the same topology.

Fig. 6 illustrates the evolution of the refractive index spectrum as a function of energy for the four binary compounds BP, BN, BBi and BAs. The values of the refractive index obtained at zero frequency n (ω=0) are grouped in Table 7. The refractive indices 3.0546, 2.1678, 4.6898 and 3.2198 of the compounds BP, BN, BBi and BAs, respectively, are determined by the FP – LAPW method, and by various theoretical and

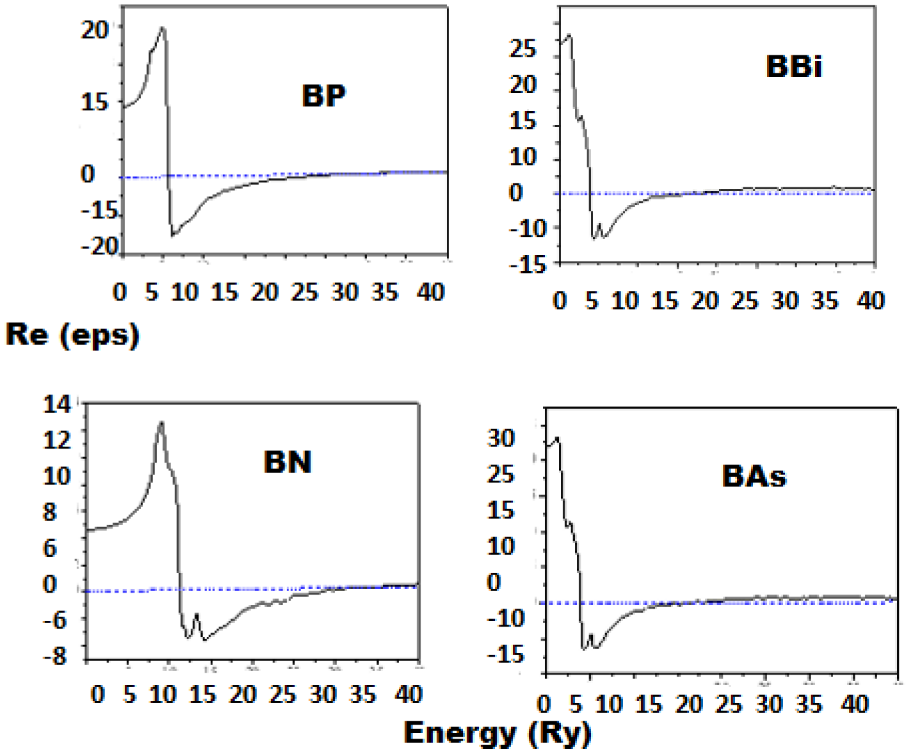

Fig.5. Variation of the real part of the dielectric function depending on energy for compounds BP, BN, BAs and BBi

Table 7: The static dielectric function ε1(0) and the static refractive index n(0) calculated for the compounds BP, BN, BBi and BAs.

	Nos calculs WC-GGA $\varepsilon_1(0)$	Autre calculs	Nos Calculs Wc-GGA n(0)	Autre calculs
BP	9.5961	8.1[a]	3.0546	3.34[a]
BN	4.6798		2.1678	
BBi	22.097		4.6898	
BAs	10.216		3.2198	

[a]Ref [91]

empirical models that we have discussed before. The results are also consistent with other theoretical and experimental studies available in the literature **[45].**

4. Conclusion

In this paper, we studied the structural, electronic, optical and thermal properties of the binary compounds BP, BAs, BN and BBi. The calculations were performed by the ab-initio method called augmented plane waves (FP-LAPW) within the framework of density functional theory (DFT).

- The structural results such as the lattice parameters and the compressibility moduli are in good agreement with the theoretical and experimental values available in the literature.
- The study of the structures of the electronic bands allowed us to conclude that the gap is indirect for the compounds BBi, BAs, BN and BP. The calculated values of the gaps of these compounds using (WC-GGA) and (mBJ) correspond well to the theoretical data.
- The most interesting for a semiconductor is its optical properties. We have determined the complex dielectric function and the refractive index. The results obtained are consistent with those of other theoretical calculations.

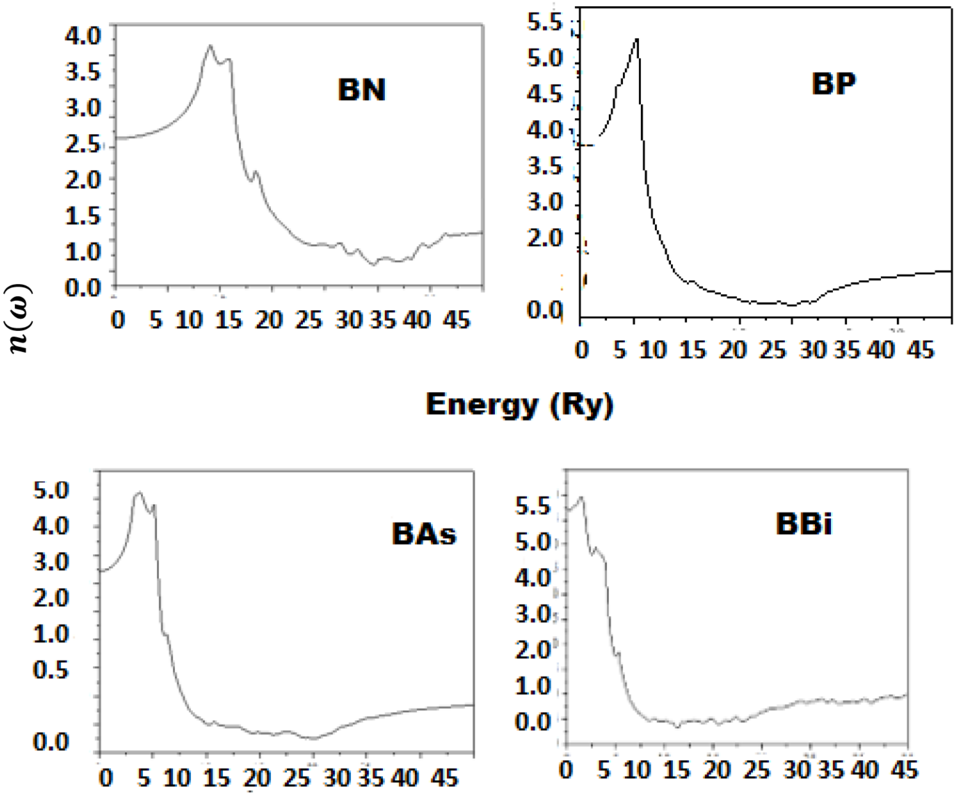

Fig 6. Variation of the refractive index depending on energy for compounds BP, BN, BAs and BBi.

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