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First-principles Study of Structural, Electronic and Optical Properties of III-arsenide Binary GaAs and InAs, and III-Nitrides Binary GaN and InN: Improved Density-functional-theory Study

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Abstract: We report results from first-principles density functional calculations using the full-potential linear augmented plane wave (FP-LAPW) method. For the exchange-correlation potential, local-density approximation (LDA) and generalized gradient approximation of Wu and Cohen (GGA-WC) have been used to calculate the structural, electronic properties of the zinc-blende GaAs, InAs, GaN and InN compounds. The alternative form of GGA proposed by Engel and Vosko (EV-GGA), and the modified Becke-Johnson exchange potential+LDA-correlation (MBJLDA) were also used for the electronic band structure and optical properties. The results obtained for structural, electronic and optical properties are compared with other computational work and experimental data. These compounds are direct band gap semiconductors, where the valence band maximum is located at the Γ^v point, and the conduction band minimum is located at the Γ^c point. In addition to that, detailed descriptions of the band structures, density of states and electronic charge densities were evaluated. The optical properties of these compounds, namely the real and the imaginary parts of the dielectric function, reflectivity and absorption coefficient were analyzed. *Copyright © 2014 IFSA Publishing, S. L.*

Keywords: FP-LAPW calculations, Electronic structure, GGA-EV, MBJLDA, Optical properties.

1. Introduction

Semiconductor materials are essential for modern electronics, many conductors based devices (such as computer and mobile phones) have become an inseparable part of everyday life. The best known and most widely used semiconductor material is silicon but many others have important applications as well [1]. This gives salutary latitude to researchers to develop new materials that have special qualities sought. However, the semiconductors III-V are rapidly emerged as the materials of choice. The III-V group elements are considered an important class of materials and this through the adjustment of their lattice parameter, energy band gap and other physical parameters that can be adjusted and controlled for obtaining a desired good optoelectronic component [2]. The III-V materials are semiconductor compounds formed from an element of the third column and an element of the fifth column of the Periodic table and have nearly all a direct gap. III-arsenide where the gallium arsenide and indium arsenide are the best known representative with a gap of 1.52 eV for GaAs [3] and 0.42 eV for InAs [4], this group has another great strength resides in the large number of alloys possible between B, Al, Ga, In and As.

Very little experimental and theoretical work has been reported in literature about the structural and electronic properties of these compounds. The gap for III-arsenide always remains less than 2.5 eV about, and we cannot consider them as wide band gap materials. The coming of new materials, such as III-nitride goes expand this family of semiconductor III-V. The III-nitrides, gallium nitride (GaN) and indium nitride (InN) are essentially candidate materials for optoelectronic applications in such photon energy [5], because they form a continuous alloy system (InGaN, InAlN and AlGaN) whose direct band gap in the cubic phase range from 0.7 eV [6,7] for InN, and 3.20 eV for GaN [3]. These nitrides of the band gap of 0.7 to 3.2 eV, can there to cover the entire spectral range from the near infrared to ultraviolet (1771 to 387 nm).

In this paper we report results of a systematic study of structural, electronic structure and linear optical properties of GaAs, InAs, GaN and InN crystals in zinc-blende. First principles calculations were performed within the density functional theory (DFT) framework [8]. The underestimation in the energy band gap performed by GGA-EV and MBJLDA was corrected by the scissor operator technique. The rest of the paper is organized as follows: in Section 2 we show our method of calculation. In Section 3 we present our results of the calculations, and discuss the linear optical properties. A summary of our work is given in Section 4.

2. Computational Details

In this work, the calculation for the structural, electronic and optical properties of zinc-blende binary GaAs, InAs, GaN and InN were performed using the full-potential linear augmented plane wave (FP-LAPW) within the framework of the density functional theory (DFT) as implemented in the wien2k computer code [9]. For the FP-LAPW calculations reported in this paper, the exchange and correlation effects were treated by using the recent form of GGA proposed by Wu and Cohen (WC-GGA) [10] and the standard local density approximation (LDA) using the scheme of Ceperly-Alder as parameterized by Pedrew-Zunger [11]. In addition we used the Engel-Vosko (GGA-EV) formalism [12] and the modified Becke-Johnson approach (MBJLDA) [3], which optimize the corresponding potential for band structure calculations. Both last approximations were developed only for calculating the energy band structure and not the structural parameters.

To achieve energy eigenvalues convergence, the plane wave expansion with an $R_{MT}xK_{MAX}$ was equal to 9, where R_{MT} is the smallest radii of the muffin-tin spheres and K_{MAX} is the cut-off for the wave function basis. The R_{MT} values (muffin-tin radii) were taken to be 2.0, 2.1 and 2.0 atomic unit (a.u) for Ga, As and In, respectively for GaAs and InAs binary compounds. In the case of GaN and InN, we chose a value of 1.83, 2.00 and 1.74 atomic unit (a.u) for Ga, In and N respectively. The maximum value for the angular momentum quantum $l_{max}=10$ is adopted for the wave function expansion inside the atomic spheres, while the charge density Fourier expanded up to $G_{max}=12$ $(a.u)^{-1}$. Self-consistent calculations are considered to have converged when the total energy of the system is stable within $<10^{-5}$ Ryd. Integrals over the Brillouin Zone were performed up to 47 k-points (grid of 10×10×10 meshes, equivalent to 1000 K-points in the entire BZ) in the irreductible BZ.

3. Results and Discussions

3.1. Structural Parameters

The equilibrium structural parameters of all binaries zinc-blende were performed by fitting the total energy versus volume to the Murnaghan's equation of states [13, 14].

$$E(V) = E_0 + \frac{B_0 V}{B_0^{'}}\left(\frac{\left(V_0/V\right)^{B_0^{'}}}{B_0^{'}-1}+1\right) - \frac{B_0 V_0}{B_0^{'}-1}, \qquad (1)$$

where E_0 is the equilibrium energy, B_0 the bulk modulus, B_0' is the first derivate of B_0. The equilibrium volume, lattice constants, bulk modulus B and its first pressure derivative B' were calculated within de GGA-WC and LDA approximations. We calculated the total energy versus unit cell volume of GaAs, GaN, InAs and InN compounds as shown in Fig. 1. From the energy volume curves obtained, the equilibrium volume, bulk modulus and the derivatives of the bulk modulus are obtained and listed in Table 1. This table displays the obtained values for the structural properties compared with previous experimental data and other calculation results. We analyzed these results we found a quite good agreement between our results and the available published works. We note from our results that the calculated lattice constant within the LDA is lower than the experimental value by about 0.5691 % for GaAs and 0.7711 % for GaN. A low difference was also noticed for InAs and InN, only 0.1540 % and 0.6706 % compared to the experimental value for InAs and InN, respectively. While the calculated values with GGA-WC are 0.4450 % larger for GaAs, 0.1777 % for GaN, 0.9128 % for InAs and 0.3032 %

larger for InN, which is due to the general trend of these approximations, the LDA underestimate the lattice constant while the GGA overestimate it. Moreover, we also calculated the bulk modulus B and its first derivative B', we remark from these that the calculated bulk lattice constant obtained from GGA-WC and LDA calculations are also shown to be in good agreement with the available experimental and other reported theoretical results.

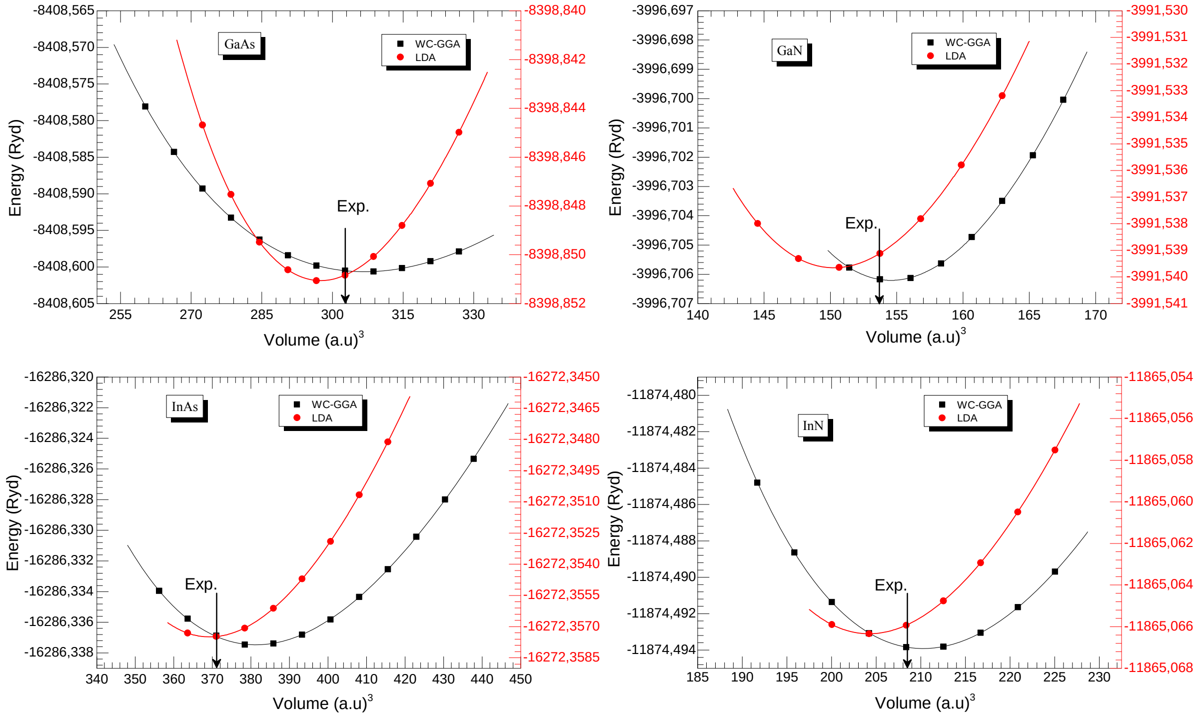

Fig. 1. Total energy versus volume using GGA-WC and LDA approximations for GaAs, GaN, InAs and InN binary compounds.

Table 1. The lattice constant a, volume V, the bulk modulus B and its first derivative B' of GaAs, GaN, InAs and InN compounds compared to experimental and theoretical values.

Compounds	**Method**	***a (Å)***	***V (a.u)*^{3}**	***B (GPa)***	***B'***
GaAs					
Present work	FP-LDA	5.6079	297.5369	74.0432	4.8795
	FP-GGA(WC)	5.6654	306.7886	69.6748	4.3434
Experiment		**5.640 [15]**		**77.00 [15]**	
Other theoretical works		5.608 [16]	297.606 [16]	75.20 [16]	4.814 [16]
		5.666 [17]		69.60 [17]	
		5.580 [18]		74.53 [18]	
GaN					
Present work	FP-LDA	4.4653	150.2600	206.5215	4.7725
	FP-GGA(WC)	4.5080	154.5602	193.2144	4.8924
Experiment		**4.50 [4, 19]**		**190 [27]**	
Other theoretical works		4.48 [20]		192.564 [20]	4.963 [20]
		4.50 [21]			
InAs					
Present work	FP-LDA	6.0267	369.2939	59.8387	4.5114
	FP-GGA(WC)	6.0911	381.2687	55.1203	4.7349
Experiment		**6.036 [16, 22]**		**58.00 [16]**	**4.79 [16]**
Other theoretical works		6.015 [23]		60.30 [23]	4.90 [23]
		5.956 [24]		65.70 [24]	
		6.191 [25]		48.68 [25]	
InN					
Present work	FP-LDA	4.9466	204.2016	147.2566	4.8909
	FP-GGA(WC)	4.9951	210.2707	136.5642	4.7334
Experiment		**4.98 [4, 26]**		**137 [27]**	
Other theoretical works		4.957 [24]		183.3 [24]	

3.2. Electronic Properties

The band structure of the constituents GaAs, GaN, InAs, InN in the zinc-blende phase, the total and partial density of states (DOS) and the electronic charge densities have been calculated at the theoretical equilibrium lattice constant.

The calculated electronic band structure along high symmetry lines of the first Brillouin zone for all compounds and the total densities of state using MBJLDA approximation are presented in Figs. 2 and 3. All zinc-blende binaries are direct band gap because the top valence and the bottom conduction are found at Γ point. From Table 2, the results by using GGA-WC approximation indicate values of 0.341 and 1.650 eV for GaAs and GaN, respectively, while the LDA gives a band gap of 0.463 and 1.915 eV for GaAs and GaN. In the case of InAs and InN, GGA-WC and LDA methods gave practically a zero band gap (0eV). A known effect of LDA and GGA-WC is the underestimation of the band gap of semiconductors. In order to obtain a more accurate band structure, we have calculated a band gap of all binaries by using another functionals such as the EV-GGA and the MBJLDA. In EV-GGA, Engel and Vosko have proposed an alternative form of generalized gradient approximation which was obtained by optimizing the exchange-correlation potential [12]. The calculated electronic band gaps with EV-GGA are presented in Table 2. The band gap has been evaluated to be 0.968, 2.293, 0.224 and 0.114 eV for GaAs, GaN, InAs and InN respectively, which are in reasonable agreement with other calculations, but still far from the experimental values. We calculated the band gap by using the modified Beche-Johnson combined with the local density approximation (MBJLDA) in order to obtain a best value of the gap energy (closer to experiment). The detail of this approach is well explained in ref. 3.

Now we present the calculated partial and the projected density of states (DOS) using EV-GGA and MBJLDA approximations. The predicted density of states (DOS) shows not much difference between GGA-WC, LDA, EV-GGA and MBJLDA. Because of this similarity, we analyzed and presented in this section only the DOS obtained with the MBJLDA. From Figs. 2 and 3, we remark that for all compounds, the valence band region is divided into three sets that we will call low-, intermediate-, and higher-energy band.

To obtain a deeper understanding of the electronic structure of our compounds, we analyzed the contribution of each atomic character in a series of bands by decomposing the total density of states into contributions of *s*, *p* and *d* orbitals (Figs. 4 and 5). For GaAs and InAs, the valence band between -14.8 to 14.4eV is formed by d orbitals of Ga and In atoms, for GaN and InN compounds, the contribution of d states of Ga, In and N atoms appears clearly in this region (from -16 to-14.4eV). The intermediate energy band in the range of -12.4 to -9.8 eV comes from As_s orbitals for GaAs and InAs compounds, while

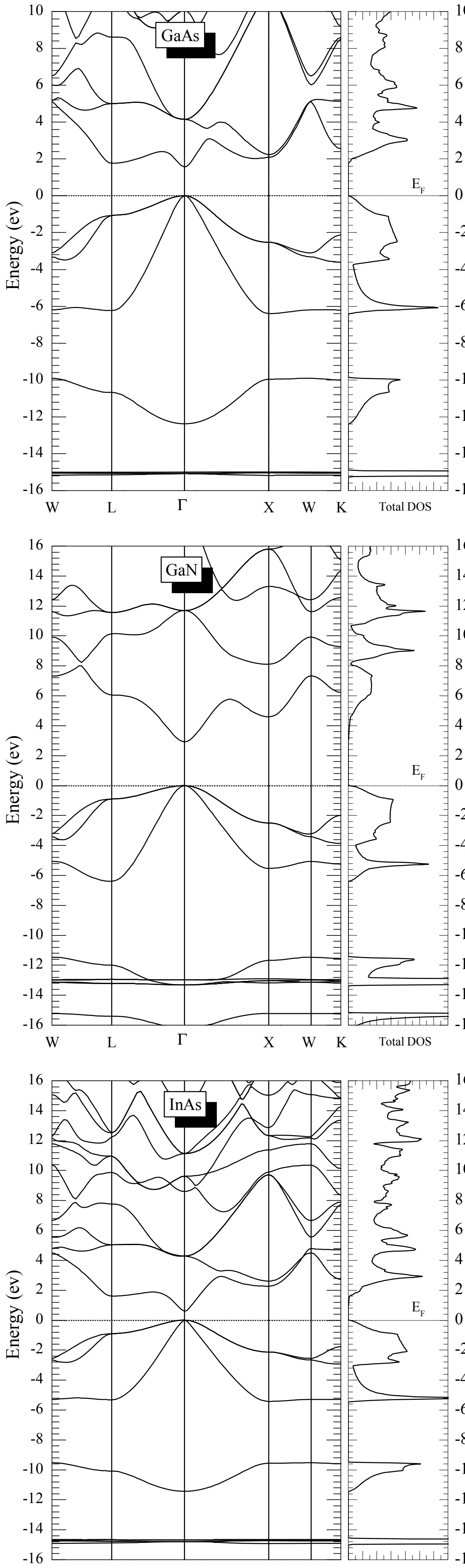

Fig. 2. Calculated band structure and total density of states for GaAs, GaN and InAs using MBJLDA.

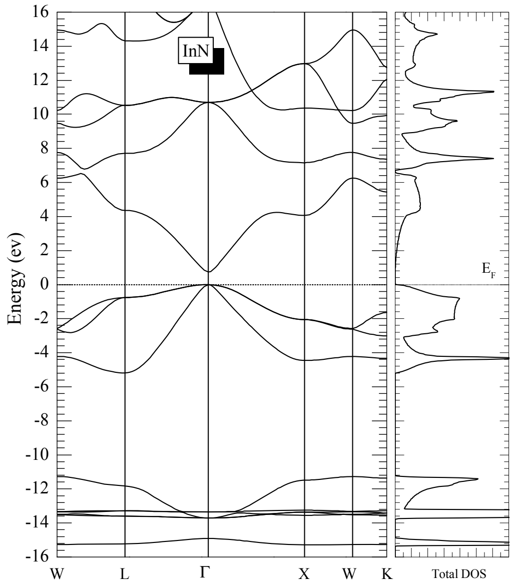

Fig. 3. Calculated band structure and total density of states for InN using MBJLDA.

Table 2. The energy band gap (Eg) for GaAs, GaN, InAs and InN.

Compounds	Computationnel method	Eg (ev)
GaAs		
Present work	GGA-WC	0.341
	LDA	0.463
	GGA-EV	0.968
	MBJLDA	1.560
Experiment		**1.520 [3]**
Other theoretical works	GGA	0.51 [16]
	LDA	0.28 [16]
	GGA-EV	0.97 [28]
	MBJLDA	1.64 [3]
GaN		
Present work	GGA-WC	1.650
	LDA	1.915
	GGA-EV	2.293
	MBJLDA	2.933
Experiment		**3.20 [3, 19]**
Other theoretical works	LDA	1.80 [29]
	LDA	1.63 [3]
	MBJLDA	2.81 [3]
InAs		
Present work	GGA-WC	0.00
	LDA	0.00
	GGA-EV	0.224
	MBJLDA	0.593
Experiment		**0.420 [4]**
Other theoretical works	LDA	0.00 [30]
	GGA	0.00 [16]
	GGA-EV	0.40 [16]
InN		
Present work	GGA-WC	0.00
	LDA	0.00
	GGA-EV	0.114
	MBJLDA	0.741
Experiment		**0.7 [6,7]**
Other theoretical works	LDA	0.00 [31]
	GGA	0.00 [31]

for GaN and InN, the dominance comes from d orbitals of Ga and In atoms in range -13.8 to -11.6 eV. Near the gap, the higher-energy valence band is divided into two sub-bands, the first sub-band energy from -6.4 to -4 eV for GaAs and GaN is a constitution of s and p characters of Ga, As and N atoms, the second from -3.8 to 0 eV is formed by p states of Ga and As atoms in the case of GaAs compound, while for GaN, this second sub-band is formed of mixture of p and d states of Ga and N atoms. For InAs and InN, we observed that the sub-band energy range from -5.4 to -3 eV contain a mixture of In-s and As-p for InAs and In-s and N-p for InN, while for the energy range of -3 eV up to Fermi energy (E_F), the region is dominated by p states of In, As and N atoms, with a small contribution comes from In-d orbital for InN.

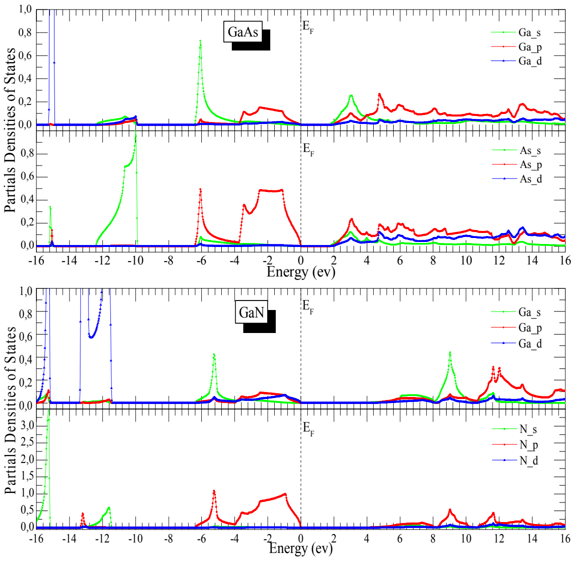

Fig. 4. Partial density of states for GaAs and GaN.

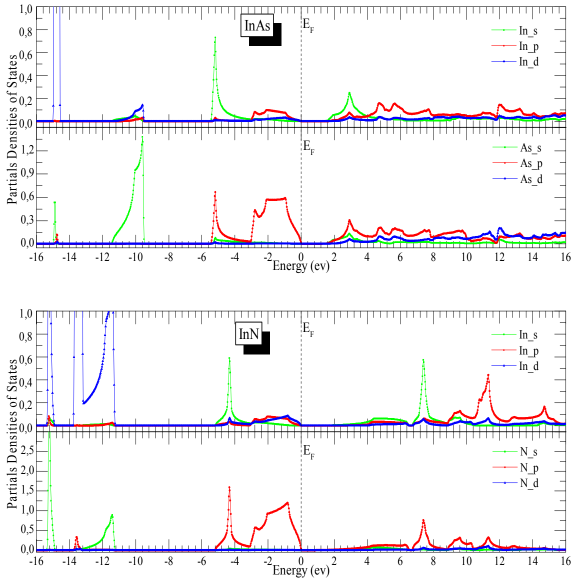

Fig. 5. Partial density of states for InAs and InN.

One of the more obvious ways to analyze the nature of the chemical binding of a material is to simply inspect the calculated charge density. The bonding properties of the investigated compounds were explained by the investigation of the electronic charge density contours in the (110) plane as shown in Fig. 6. We have presented only the MBJLDA calculations of the electronic charge densities of our binary compounds, we presented here not only the 2D contour, but also the distribution of the electronic charge density in 3D, to better visualize the contribution of electrons for each atom. The contour plots show more covalent bonding between Ga-As and In-As, while for GaN and InN compounds, pure covalent bonding is not known to exist, these compounds have a degree of ionic bonding between Ga-N and In-N which depends on the Pauling electronegativity difference of Ga(1.81), In(1.78) and N(3.0) atoms. Thus, Arsenic changed with Nitride, the ionic character becomes significant, with a polar covalent bond for all atoms.

3.3. Optical Properties

Several areas where the light reacts with the matter are obviously of practices interest. Studies of the optical properties of solids have been proven to be a powerful tool for understanding the electronic and atomic structure of these materials [32]. Given that our study are to develop an understanding of the optical properties and predict the possibility of finding compounds desirable for use in optical applications. The optical properties can be described by means of the dielectric function ε(ω) that can be used to explain the response linear crystal system for electromagnetic radiation. The imaginary part of the dielectric function in the long wavelength limit has been obtained directly from the electronic structure calculation, using the joint density of states and the optical matrix elements. The real part $\varepsilon_1(\omega)$ of dielectric function can be derived from the imaginary part $\varepsilon_2(\omega)$ by the Kramer-Kronig relationship. The dielectric function is given by

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega) \tag{2}$$

The imaginary part $\varepsilon_2(\omega)$ of dielectric function derives from the appropriate momentum matrix, is given by [33].

$$\varepsilon_2(\omega) = \frac{e^2\bar{h}}{\pi m^2\omega^2}\sum_{v,c}\int_{BZ}\left|M_{cv}(k)\right|^2 \delta[\omega_{cv}(k)-\omega]d^3k \tag{3}$$

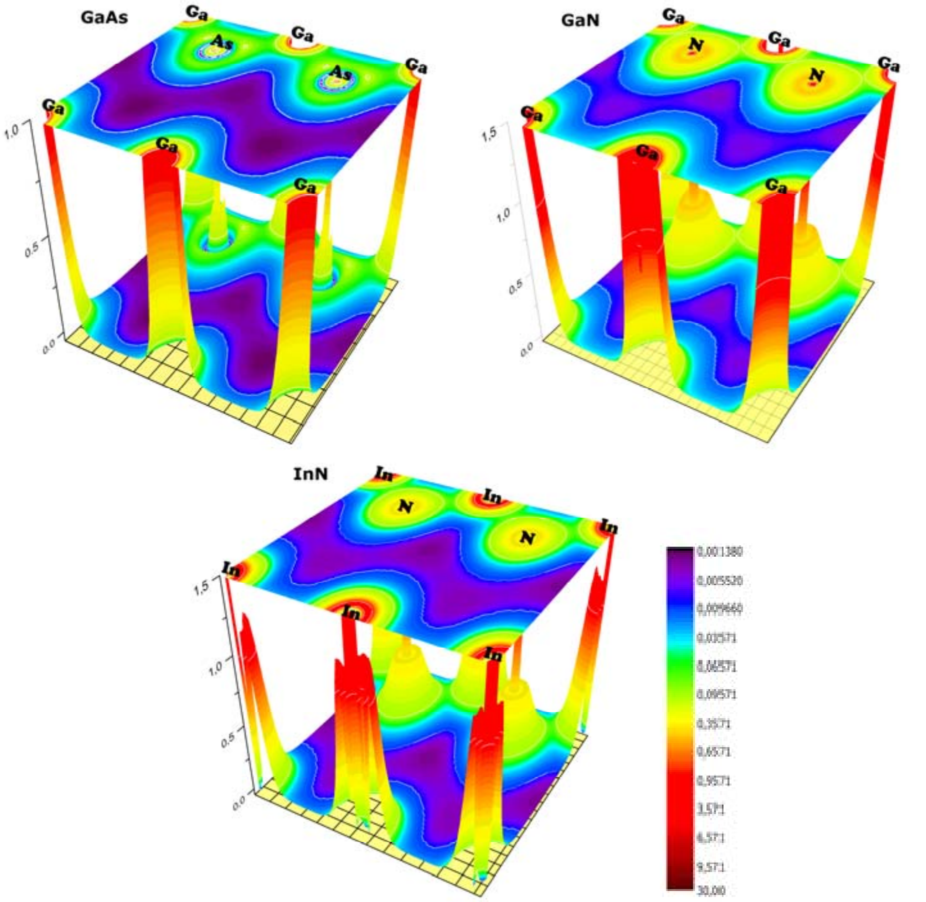

Fig. 6. The 3D bonding charge density distributions and contours projected for GaAs, InAs, GaN and InN using MBJLDA.

The integral is over the first Brillouin zone [17], $M_{cv}(k)=\langle u_{ck}|e.\nabla|u_{vk}\rangle$ is the momentum elements, where e is the potential vector defining the electric field.

The real part $\varepsilon_1(\omega)$ of dielectric function can be obtained from $\varepsilon_2(\omega)$ by the Kramer-Kronig transformation [34].

$$\varepsilon_1(\omega)=1+\frac{2}{\pi}p\int_0^\infty\frac{\omega'\varepsilon_2(\omega')}{\omega'^2-\omega^2}d\omega' \qquad (4)$$

With the Knowledge of both parts of the dielectric function, we can easily determine the reflectivity $R(\omega)$ and the absorption coefficient $\alpha(\omega)$.

$$R(\omega)=\left|\frac{\varepsilon^{1/2}(\omega)-1}{\varepsilon^{1/2}(\omega)+1}\right| \qquad (5)$$

$$\alpha(\omega)=\sqrt{2}\omega\left[\left(\sqrt{\varepsilon_1^2(\omega)+\varepsilon_2^2(\omega)}\right)-\varepsilon_1(\omega)\right]^{1/2} \qquad (6)$$

GaAs and InAs binaries crystallize under normal conditions in the cubic zinc-blende (ZB) lattice (space group T_d^2-$F\bar{4}3m$) [35]. This symmetry group has one component of the dielectric tensor. Gallium nitride and indium nitride crystallize under normal conditions in the (hexagonal) wurtzite lattice (space group C_{6v}^4-$P6_3mc$). Work on zinc-blende nitrides is motivated by the potential advantages that these materials would offer for electronic and opto-electronic applications, compared to the hexagonal nitrides [36]. We use the ZB structure for all concerned compounds.

In order to calculate $\varepsilon_1(\omega)$, one needs to have a good representation of $\varepsilon_2(\omega)$, a dense mesh of uniformly distributed k-points is required. Hence the Brillouin zone integration was performed with 560 k-points in the irreducible part of the Brillouin zone. Since all our binary have cubic symmetry, we need to calculate only one dielectric tensor component to completely characterize the linear optical properties. We should mention that we have performed the linear optical calculations with GGA-WC, LDA, GGA-EV and MBJLDA, but we present only the figures corresponding to the GGA-EV and MBJLDA calculations. The half-width lorentzian broadening [37] is taken to be 0.05 for all our compounds, using GGA-EV and MBJLDA. We also note that the scissor operator [38] was taken into account in our calculation of optical properties, this value is the difference between the calculated energy gap and measured one.

Fig. 7 displays the calculated imaginary part of the electronic dielectric function $\varepsilon(\omega)$ of our compounds within GGA-EV and MBJLDA for a radiation up to 15 eV for GaAs and InAs, and 20 eV for GaN and InN.

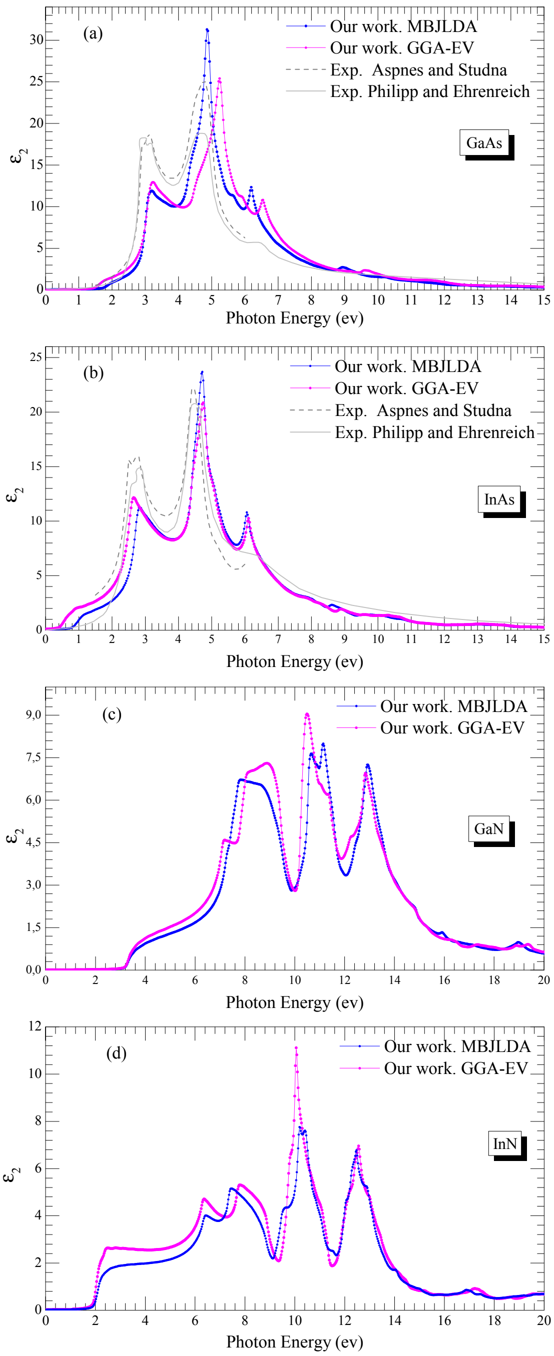

Fig. 7. Imaginary part of the dielectric function for GaAs, InAs, GaN and InN within GGA-EV and MBJLDA approximations.

We report in the graphs 7(a) and (b), the experimental results found by Aspnes and Studna [39], and Philipp and Ehrenreich [40]. Our calculated $\varepsilon_2(\omega)$ for GaAs and InAs with GGA-EV and MBJLDA shows better agreement with the experimental data [39, 40].

As it can be seen in Fig. 7, the edges of optical absorption of the dielectric function $\varepsilon(\omega)$ occurs at 1.41 and 0.42 eV for GaAs and InAs with GGA-EV and 1.7 and 0.783 eV with MBJLDA. For nitrides binary (GaN and InN), the absorption threshold takes values of 3.19 and 1.93 eV for GaN and InN, the same values were reported for MBJLDA. These critical points are Γ_{15v}-Γ_{1c} splitting which gives the threshold for direct optical transitions between the highest valence and the lowest conduction band. As a general observation, for arsenide binaries, the curves 7(a) and (b) show three peaks in the energy ranges between the absorption threshold and 8 eV of photon energy. These three critical points occurs at about 3.14, 4.88 and 6.20 eV for GaAs with MBJLDA, and 3.19, 5.25 and 6.52 eV with GGA-EV, which are correspond to the electronic transitions (L_{3v}-L_{1c}), (X_{5v}-X_{3c}) and (L_{3v}-L_{3c}) respectively. A slight difference was remarked by comparing our calculations with experimental results. The positions of 2.81, 4.71 and 6.08 eV occupy the three critical points for InAs with MBJLDA, and 2.62, 4.76 and 6.12 eV with GGA-EV, the Aspnes and Studna results on InAs, shows the peak positions at about 2.7, 4.4 and 6.1 eV. This could be interpreted by the underestimation of the band gap of semiconductor compounds, hence the uses of the scissor operator [38] to correct the band gap calculated theoretically, and bring it to the experimental value of the corresponding materials. In the other hand, still with the arsenide binaries, by replacing Ga by In, the peak height was reduced, this change is attributed to the reduction of the band gap.

For nitride binaries, the calculated $\varepsilon_2(\omega)$ shown in Fig. 7(c) and (d) has three groups of peaks. For GaN, it be clearly seen from graphs that the first peak groups is presented in the range energy from the absorption threshold up about 10 eV of photon energy, contains two peaks at 7.80 and 8.66 eV with MBJLDA and with GGA-EV we note three peaks at 7.17, 8.09 and 8.91 eV. The major peak corresponds to X_{5v}-X_{1c} electronic transition. The second group presents its major peak at the value of 10.84 eV with GGA-EV and 11.14 eV with MBJLDA for GaN, while for InN, this major peak is presented at the values of 10.05 eV and 10.20 eV with GGA-EV and MBJLDA respectively. This second major peak corresponds to electronic transition X_{5v}-X_{3c}. The major peak of the third group is found for GaN at 12.85 and 12.93 eV within approximations, 12.55 and 12.50 eV for InN, which corresponds to L_{3v}-L_{1c} electronic transition. For all our materials, the main origin of these peaks is attributed to the interband transition from the occupied Ga (In)_*s/p/d* and As (N)_*p* states to unoccupied Ga (In)_*s/p* and As (N)_*p*.

Fig. 8, shows the evolution of the real part $\varepsilon_1(\omega)$ of dielectric function $\varepsilon(\omega)$, the calculated static dielectric constant $\varepsilon_1(0)$ for arsenide binaries are 9.85 and 9.58 for GaAs with GGA-EV and MBJLDA respectively. A slight difference is noted with the experiment results [40]. For InAs, the value i.e. static dielectric constant $\varepsilon_1(0)$, is presented at about 11.26 and 9.94 with GGA-EV and MBJLDA, the result of 11.67 is reported with the experimental measurement [40].

For nitrides binaries we note values of 4.75 and 4.48 by GGA-EV and MBJLDA for GaN, and 5.76 and 5.09 for InN.

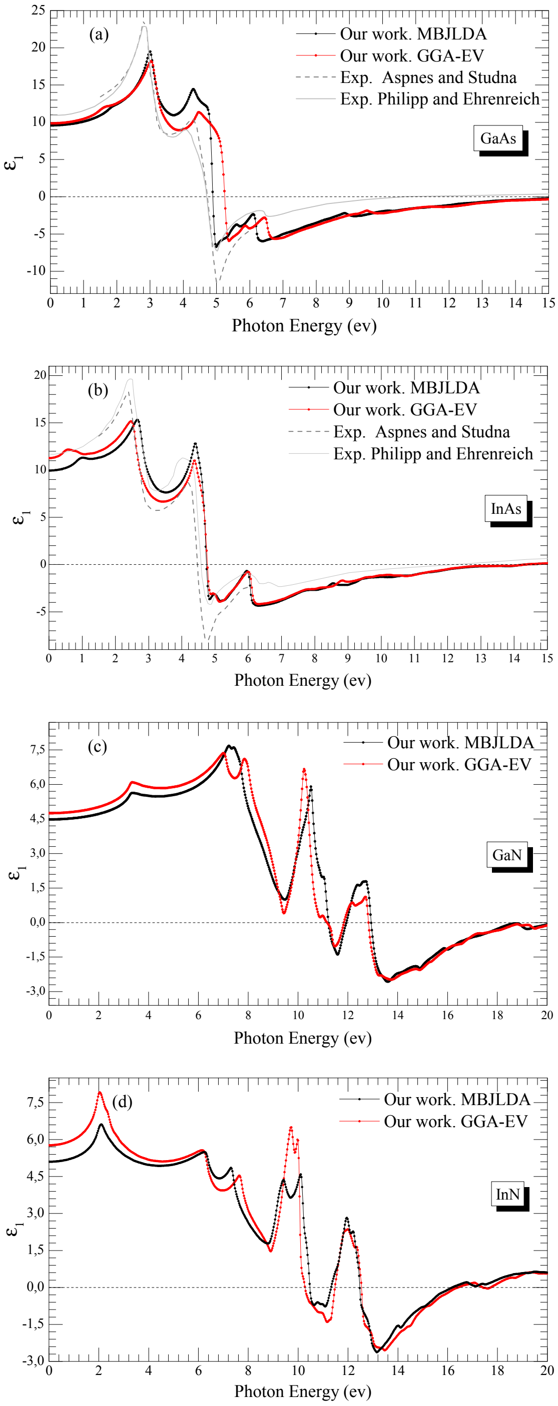

Fig. 8. Real part of the dielectric function for GaAs, InAs, GaN and InN compounds using GGA-EV and MBJLDA.

As it can be seen, the calculated values with GGA-EV are greater than that by MBJLDA, indicating that the obtained $\varepsilon_1(0)$ has inversion relationship via Penn model [41] based on the expression $\varepsilon(0)\approx 1+(\hbar\omega_p/E_g)^2$.

The reflectivity spectra for arsenide and nitride binaries are shown in Fig. 9.

The maximum reflectivity values for GaAs are 62 and 60.3 % located at about 4.95 and 5.34 eV of photon energy with MBJLDA and GGA-EV, which are in the ultraviolet spectra.

The good agreement with experiment results [39, 40] is found. For InAs, we note the values of 56.83 and 55.18 % occur at 4.8 eV. In the case of nitride compounds such as GaN and InN, the maximum reflectivity spectrum is found around 50 %, we remarked that the photon energies of these maxima reflectivity are higher than that of arsenide binaries, this is due to the change of arsenide by the nitride elements.

The calculated wavelength dependences of the absorption coefficient for GaAs, InAs, GaN and InN are plotted in Fig. 10.

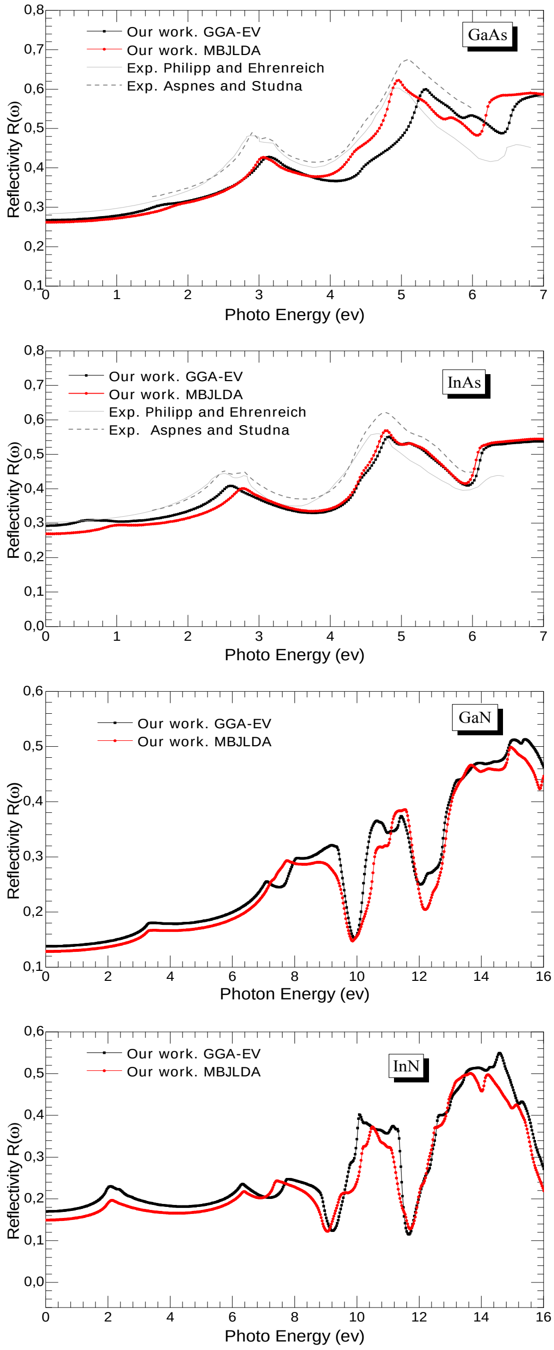

Fig. 9. Reflectivity variation for GaAs, InAs, GaN and InN compounds using GGA-EV and MBJLDA.

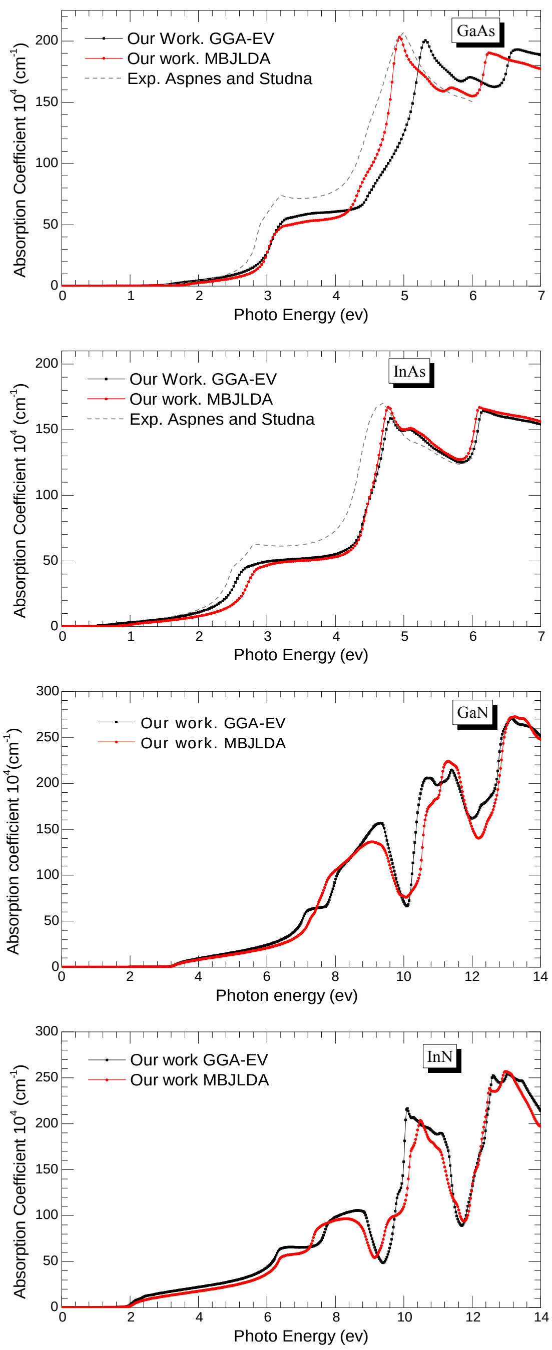

Fig. 10. The absorption coefficient as a function of photon energy of GaAs, InAs, GaN and InN compounds using GGA-EV and MBJLDA.

The experimental results reported from [39] for GaAs and InAs were added for comparison with our calculated values. A zero absorption coefficient for all compounds was observed for photons possessing energies below the band gap (IR region). We remark also that the absorption coefficient is too low in the visible region, and reaches its maximum value in the UV (Ultra-Violet) region, an MBJLDA value of 203 and 167×104 cm^{-1} at photon energy of 4.93 and 4.77 eV were found for GaAs and InAs, respectively; this was in good agreement with experiment results [39]. For nitrides binary we note the values of 272 and 256×104 cm^{-1} for GaN and InN at energy of 13.26 and 12.96eV, respectively. However, the replacement of As by N, increases the peak height, this increase is attributed to the variation of band gap.

4. Conclusions

In summary, we have made the first principles calculations to study the fundamental properties of III-arsenide and nitrides binary compounds GaAs, InAs, GaN and InN by using the density functional theory within GGA-WC and LDA approximations. Our calculated parameters are in quite good agreement with previous theoretical and experimental data. In addition, we used two others new developed approximations as the GGA-EV and MBJLDA which usually provide a good prediction of the band structure. The calculated energy gap using GGA-EV are in reasonable agreement with experimental one. The MBJLDA method seems to give a better estimation of the band gap. The total and partial densities of state and electronic charge densities were obtained and analyzed. We present results for the imaginary and real parts of the dielectric function, however the replacement of Ga by In for III-arsenide and III-nitride binary, reduced peak height, this change is attributed to reduction of the band gap. From the real and imaginary parts of the dielectric function, the reflectivity and absorption spectrum were obtained and discussed in detail.

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