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First-principles calculations on structural, electronic and magnetic properties of V doped GaAs semiconductor

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ABSTRACT

The aim of this study is investigate different physical properties of novel diluted magnetic semiconductors Ga1-xVxAs (x = 0.25, 0.50 and 0.75) to find our results we based on the method on linearized augmented plane waves under the frame work of density functional theory, and for more accurate results we used as exchange correlation energy approximation (TB-mBJ). As physical properties we highlighted the structural, electronic and magnetic properties for the three mentioned alloys. As we found, the both alloys Ga1-xVxAs (x = 0.25 and 0.50) show a semiconductors behavior while the third one Ga1-xVxAs (x =0.75) indicate that a half-metallic which has a total magnetic moment equal to 6 μB (mainly due to V-d states) and there is a small local magnetic moment on the Ga and As sites. Importantly, behavior which make it a good candidate for spintronic devices.

Key words : Ab initio calculations, Electronic properties, Doped semiconductors , DFT FPLAPW method.

1. INTRODUCTION

The use of III-V compound semiconductors for optoelectronic technology has attracted the attention of the solid-state physics community due to their novel physical properties. In particular, several optoelectronic devices, such as solar cells, semiconductor lasers, and light - emitting diodes are made from III - V compounds, such as GaAs, InP, GaN, and GaSb. Therefore, a great effort has been devoted to the study of these compounds. The doping of non-magnetic semiconductor materials by a transition metal offers the possibility of studying both the degree of freedom of charge and of the electron spin of these doped materials and which may play a promising role in applications spintronics [1 3]. In this stage, several studies have been launched to prove the doping effect on the III - V compounds, among these studies we find the doping of a considerable quantity of Mn atoms in InAs and GaAs who have already demonstrated their historic success in setting up spintronic devices [4,5].

Therefore, there are several theoretical studies that have led to predictions the stability of HM ferromagnetism of doped materials in which, such as, we find the doping of GaN by Mn [6], V doped by CdTe [7], thanks to which an appreciable number of HM materials have been obtained experimentally [8, 9].

Much research has been devoted to probing the half-metallicity and the ferromagnetic order for their influence on various physical properties [10,11]. However, it is important for the practical application of spintronic devices to study materials for HM ferromagnetic behavior having compatibility with important III - V and II - VI compound.

Numerous theoretical and experimental studies have been directed towards magnetic semiconductors exhibiting spin polarization with Tc above room temperature [12,13]. In these materials, the sp-d exchange interaction is responsible for HM ferromagnetism for doped semiconductors and diluted magnetic semiconductors (DMS) [14,15].

Indeed, numerous studies, both experimentally and theoretically [16]. In order to identity the FM behaviour using ab-initio electronic structure calculations based on the generalized gradient approximation. GaAs is a direct bandgap semiconductor (Eg = 1.42 eV [17,18] and when doped with transition metals, a FM ordering appears at room temperature.

The aim of this study is to report on the study of the first principles of structural properties; Electronic and magnetic GaAs stabilized by various V concentrations. From the results, we observe that V doping transforms semiconductor GaAs with a semi-metallic character. By increasing the concentration of V0.75, the ground state changes from antiferromagnetic to FM. Therefore, in this study, we investigated the relationship between the structure and the

magnetic properties of V-doped GaAs structures. Recently, in-depth studies have been studied to control the properties of (DMS) as AlP doped in Vanadium and in Mn doped in GaAs. We of course believe that our products will be good candidates for spintronic applications.

In this work, we first present an introduction on the usefulness of using magnetic semiconductors and the importance of GaAs materials. After we define the calculation method and the approximation used in the DFT formalism and at the end the results of our studies of each property and a conclusion on our study.

1.1 Computational Methods

In this study we used the full potential linearized augmented plane waves method (FP-LAPW) under the framework of density functional theory (DFT) [19], implemented in Wien2k code [20]. the exchange correlation potential that used is the Generalized Gradient Approximation (GGA) proposed by Perdew, Burke and Ernzerhof (PBE96) [21]. It is well known that the standard method of DFT (GGA) underestimates the calculation of the energy gaps of semiconductors and overestimates hybridization between electronic states. In order to overcome the problem of underestimating the gap energy we used the Becke-Johnson exchange and correlation potential modified by Tran and Blaha (GGA + mBJ) [22]. Our binary compounds were doped respectively by the element of vanaduim with concentrations x=0.25, 0.50 and 0.75 these doped materials were modeled by supercells with cubic structure 1x1x1 containing 8 atoms. Doping was introduced by replacing the host atom Ga with a doping atom V, We have developed the basic function up to RMTK max = 8. The calculation was performed in a self-consistent manner with 11*11*11 k points in the reduced Brillouin zone. The cut off energy was taken equal to -6 Ry and the calculation accuracy on energy being 10 -4 Ry.

2. Results and Discussion

2.1 - Structural properties

In this work, structural optimization of the binary compound GaAs and their ternary alloys Ga 1-xVxAs (x = 0.25, 0.50 and 0.75) was calculated with the TB + mBJ approximation to obtain a minimum total as a function of the volume of the unit cell.The first step that we had start with is the calculation of the unit-cell parameter (a) and the bulk modulus (B) and its first derivative (B '). We recall that GaAs crystallizes in the Zinc-blende structure. Its experimental crystal parameter is aexp = 5.653Å. [23].

We report in Tables 1, a summary of the different values of the crystal parameters, the bulk modulus as well as its first derivative.

From the illustrated results in the table 1, contains the optimized parameters a, B and B ' where it can be clearly seen that the calculated lattice constants for GaAs demonstrate a good agreement with the other theoretical and experimental values and we showed that lattice constant decreases, where as the bulk modulus increases , which means that the ascending order of V doping concentration in the system increases its hardness.

Table 1. The results of lattice parameter a (Å) , bulk modulus B (GPa) and first derivative (B ') of the binary compound GaAs and their ternary alloys Ga 1-xVxAs (x = 0.25, 0.50 and 0.75)

Compounds	Concentration. (*x*)	*a* (Å)	*B* (GPa)	*B'*
Exp				
GaAs		5.653[a]	77.00[b]	3.36[c]
Our work				
	0,00	5,666	69,106	4,733
	0.25	5,767	74,339	6.472
$Ga_{1-x}V_xAs$	0.50	4.560	61.166	4.001
0.	0.75	5.712	63.011	3.556
Other calculations				
GaAs		5.666 [27]	69.6 [27]	
		5.58 [28]	74.53 [28]	
		5.75 [29]	61.00 [29]	
		5.668 [30]	68.782 [30]	
		5.660 [31]	68.68 [31]	

aRef[24], b Ref[25], c Ref[26],

Note that if the concentration of the doped metal increases the unit-cell parameter values become bigger. This means that the vanadium ionic radius (205pm) is considered high as that of gallium (187pm). And the bulk modulus values of the ternary alloys Ga1-xVxAs (x = 0.25, 0.50 and 0.75) are larger than that of the binary structure GaAs and this explains that the alloy interest is more .

2.2- Electronic properties

The electronic properties of GaAs are available in the literature, where the influence of V impurities on the electronic properties of this semiconductor has not been investigated.

In this part, we have calculated the structures of electronic bands, the density of states and the charge densities to predict the nature of our material Ga1-xVxAs (x = 0.25, 0.50 and 0.75).

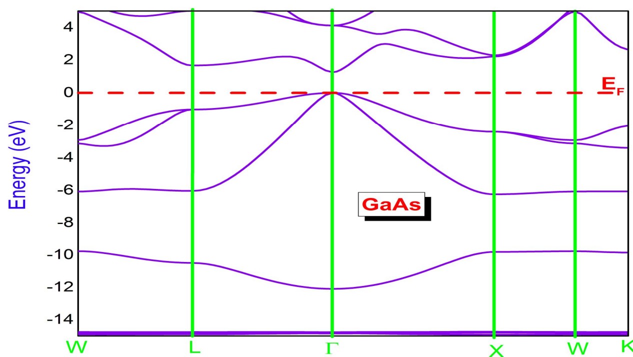


Figure 1: Band structure of the pure GaAs compound, TB + mBJ calculation

From the figure 1. Shows the calculated band structure of pure GaAs, the Fermi level is regarded as reference zero point and GaAs has a direct gap at point Γ between the valence band maximum and the conduction band minimum its value is 1.25 eV. This result is a little good agreement with the value found experimentally which is 1.42 eV [17, 18]. we also noticed that the width of the valence band is a little larger than conduction band of the order 6eV.

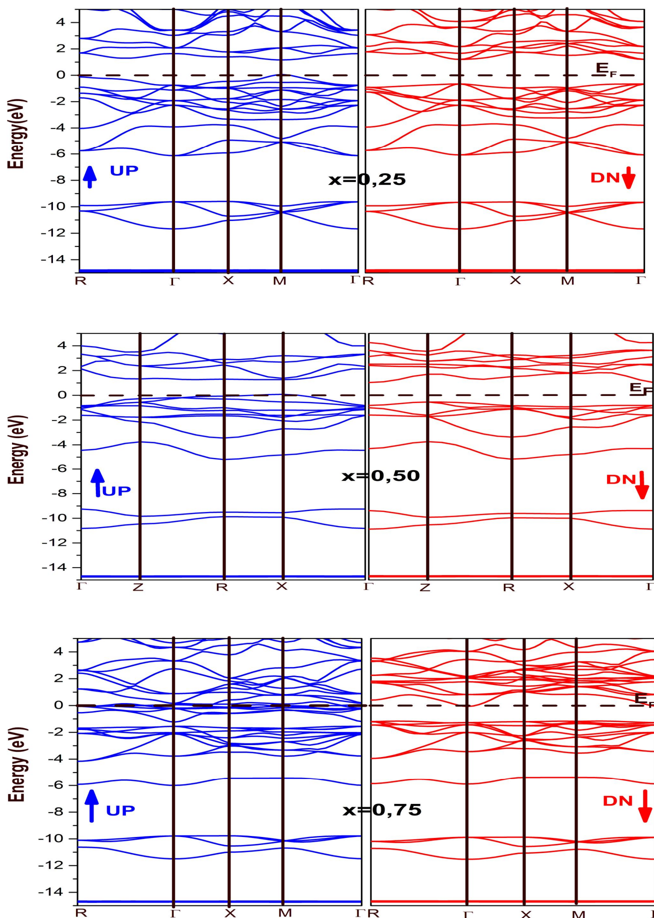
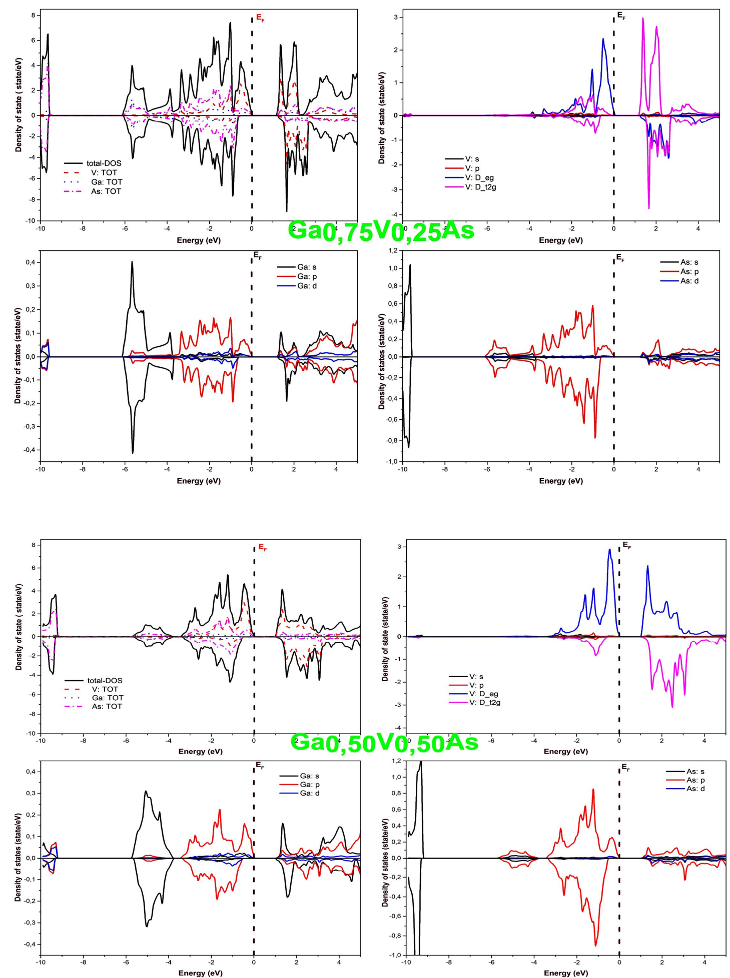


Figure 2: Band structures of the up and down spins of the $Ga_{1-x}V_xAs$ (x = 0.25, 0.50 and 0.75): TB + mBJ calculation.

The figures 2. represent the electronic band structures of the majority (spin-up) and minority (spin-down) spins along the directions of highest symmetry in the first Brillouin zone for the ternary alloys Ga 1-xVxAs (x=0.25, 0.50, and 0.75). The spin-up and spin down electronic bands are indicated by blue and red lines, respectively. It is evident from these calculations that in spin-up case, the energy bands in the valence band go across the Fermi level (EF) while in spin-down case, and it is clear that the spin-up band structure and spin-down band structure has a band gap around the Fermi level; they reside below the EF for the Ga 1-xVxAs (x=0.25, 0.50) alloys confirming their semiconductors characteristic. The values of spin-down energy band gaps Eg (eV) calculated for these alloys are 1.14eV for Ga 0.75V0.25As and 1.02eV for Ga 0.50V0.50As. According to the values found, the dopant V reduces the value of the gap of GaAs and consequently increases the magnetic moment in this material. It is noted that, in the case of doped materials, there is no previous results for sick of comparison.

From the figure 2 for Ga 0.25V0.75As shows that the spin-up band structure has a half metallic behavior but the spindown band structure has a band gap around the Fermi level.



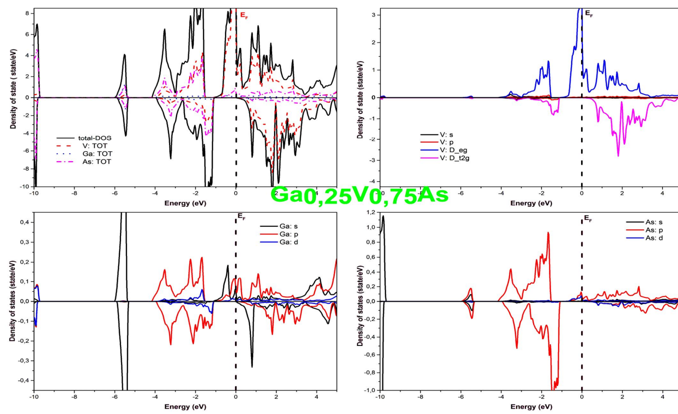


Figure 3: Total and partial DOS of the V doped GaAs compound: TB + mBJ calculation.

From the TDOS (Fig. 3) we can firstly see that there is a polarization between spin-up and spin-down states Secondly, due to the negative p–d exchange interaction (4p-As and 3d-V) there is an intersection between some states and the Fermi levels (EF) for the majority spin, but in the minority spin there is not any state at the Fermi level and we observe a gap in this channel, which confirm that the Ga 0.25V0.75As are half-metallic ompound.

The spin-up states show a semiconductor character Ga 1-xVxAs (x=0.25, 0.50) while a band gap is apparent at the Fermi level for spin down states, and, therefore, the HM characteristic of the selected ternary alloys Ga 1-xVxAs (x=0.75) in ZB phase is confirmed he densities of total states of pure and doped GaAs calculated by the approximation (TB + mBJ) and represented in FIG. 3 shows that the Fermi level passes from the top of the valence band for pure GaAs with a value of 1.25 eV at the bottom of the conduction band for Ga 1-xVxAs (x=0.25, 0.50 and 0.75) with a values are 1.14,1.05 and 0.50 respectively. The value of EF increases with the increase in the difference of valence electrons between the substitute and the dopant.

2.3- Magnetic properties

In this part, we also studied and discuss the magnetic properties such as total and local magnetic moments using the TB + mBJ functional. From the calculated values of total and local magnetic moments in Table 2 we see that the total magnetic moment per V atom in units of Bohr magneton is an integer equal to 6 μB for Ga 0.25V0.75As and (2 μB for Ga 1-xVxAs (x=0.25, 0.50)) An integer value of the Bohr magneton of the magnetic moment is a characteristic half-metallic, but semiconductor for Ga 1-xVxAs (x=0.25, 0.50) this value shows, the total magnetic moment is dependent of the V concentration.

From the negative sign of the value of the local magnetic moment of Ga, one can note that there is an antiferromagnetic interaction between the Ga and V valence spins.

The total magnetic moment values also correspond to the difference between the atomic number of the dopant V and the substituted host atom Ga. More precisely (see Table 2), the total magnetic moment comes essentially from the atom of dopant V associated with the contribution of the first neighboring atoms (As) and with a small contribution of the second neighboring atoms (Ga). We note that all the magnetic moments have the same direction, indicating a ferromagnetic coupling between the dopant and the neighboring host atoms.

Table 2 Calculated total and local magnetic moments for Ga $_{1-x}$V$_x$As using TB + mBJ

Compounds	Magnetic Moment (μB)			
	V	Ga	As	Total
$Ga_{1-x}V_xAs$ x=0.25	1.835	-0.049	0.040	2.000
$Ga_{1-x}V_xAs$ x=0.50	1.724	-0.172	0.022	2.000
$Ga_{1-x}V_xAs$ x=0.75	1.851	-0.127	0.038	6.000

Conclusion

In this paper, we employed the first-principles calculations to evaluate the structural, electronic and magnetic properties of the Ga 1-xVxAs (x=0.25, 0.50, and 0.75) in the zinc blende phase.The TB + mBJ helped us in calculating the structural properties, electronic and magnetic properties.

We can also notice that f*or* the lattice constant and bulk modulus with increasing V concentration. According to our results of electronic properties, the Ga 1-xVxAs (x= 0.75) exhibit half-metallic character behavior with 100 % spin polarization at the Fermi level and a wide semiconductor gap in the spin-up channels; where the spin-down channel has a band gap behavior. This property makes these compounds suitable for practical spintronic devices. The total magnetic moments for Ga 1-xVxAs (x= 0.75) compound come out to be an integer value confirming the HM characteristics of these The magnetism comes essentially from the d-states of impurity atom (V). Finally, the p–d hybridization reduces the local magnetic moments of V from their free space charge value (6 μB) and induces a small local magnetic moment on the non magnetic cations and anions. We hope that our predicted HM character for studied DMS compounds will motivate researchers to to remove elusive nature of half metallicity in these, experimentally.

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