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DFT Investigations of Structural and Electronic Properties of Gallium Arsenide (GaAs)

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Abstract. First principles calculations for structural and electronic properties of GaAs have been reported using a full potential linearized augmented plane wave (FP-LAPW) scheme of calculations developed within density functional theory (DFT). We use in this study local density approximation (LDA), Perdew-Burke-Ernzerhof parameterized generalized gradient approximation (PBE-GGA), Wu-Cohen parameterized GGA (WC-GGA) executed in WIEN2k code. In addition, to calculate band structure with high accuracy we used modified Becke-Johnson exchange potential (MBJ) + LDA approach. Our calculated lattice constant with GGA-WC is in good agreement to experimental value than LDA and PBE-GGA. Whereas our calculations for the band structure show that MBJ+ LDA approach gives much better results for band gap value as compared to other exchange correlation approaches.

Keywords: Density functional theory, local density approximation, gradient and other corrections, III-V semiconductors, Electronic structure calculations.

PACS: 71.15.Mb, 71.55.Eq, 74.20.Pq.

INTRODUCTION

Exploring the physical properties of materials with high accuracy in short time and reduced cost is one of the most attractive and valuable aspect of computational study of material science over the experimental study. Another intriguing aspect of simulation techniques is the prediction of the likely properties of materials that yet not explored experimentally. On the other hand, in the present era, rapid advances are taking place in the field of technology and outstanding experimental spectroscopic and microscopic techniques have been developed particularly with the advancement in laser technology to probe materials properties on a large scale, investigations of the atomic scale properties of the complex materials and their exploitation is even though a difficult and tricky one. In such a situation the computational techniques play a vital role in the fundamental understanding of required properties in atomic limits with great accuracy in short time. Motivated by these charismatic features of computer simulations, we present some calculations related to fundamental properties of GaAs using DFT [1, 2] based computational approach.

GaAs one of III-V compound semiconductor that exhibit direct band gap has attracted much attention of researchers due its potential application in the field of optoelectronic and microelectronic devices like lasers, photovoltaic cells, photo detectors, modulators, filters, integrated circuits and light emitting diodes. Thanks to its small electrons effective mass, it can be exploited to fabricate ultra fast transistors [3]. Although, due to its crucial nature industrial applications, it has been widely studied both experimentally and theoretically [4-18], a fundamental understanding of its physical properties is still in demand of this novel material. At ambient temperature and pressure GaAs exists in zinc-blende phase with experimental lattice constant 5.65 A^0 [5, 6].

Motivated by the available literature on GaAs, we carried out calculations for structural and electronic properties of GaAs in its stable zinc-blende phase using full potential linearized augmented plane wave method (FP-LPAW) designed within DFT. The rest of our paper is arranged in such a way that in section 2, details of our computational method has been given, in section 3, we briefly discussed our results, where in section 4, a conclusion of our work has been given.

COMPUTATIONAL DETAILS

In the present work we investigated the structural and electronic properties of GaAs at GGA-WC [19]; GGA-PBE [20] and LDA [21] level by FP-LAPW method based on DFT [1, 2]. In addition to the above mentioned exchange correlation potentials we also use modified Becke-Johnson potential (MBJ) [22] for the calculation of electronic structure implemented in the WIEN2k code [2].

Though calculation of electronic structure of solid material is a complex many body problem, DFT is an efficient and accurate tool for such type of systems.

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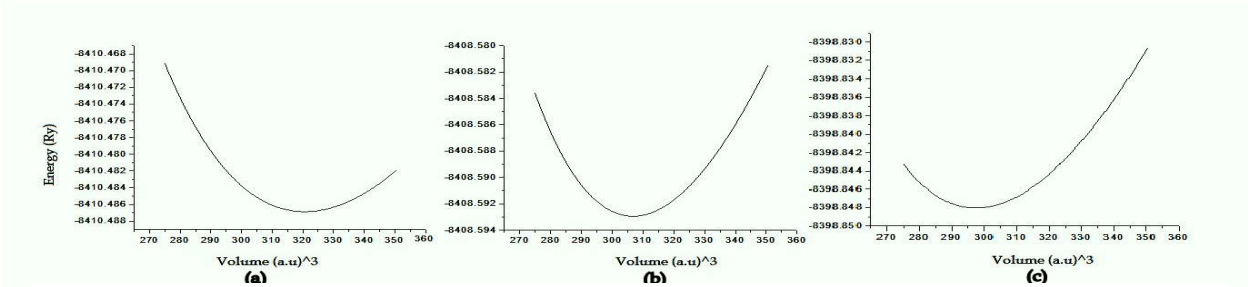

FIGURE 2. The optimized volume curves have been shown the volume of the unit cell is plotted against energy. (a), (b), (c) shows the E-V curves for GGA-PBE, GGA-WC and LDA respectively. For E-V curves the data is fitted in the Birch Mornaghan equation of states.

In this approach many body problem of an electron gas is mapped into a set of one-electron reference system as;

$$\left[-\frac{1}{2}\nabla^2 + V_{ext}(\vec{r}) + V_C\left[\rho(\vec{r})\right] + V_{xc}\left[\rho(\vec{r})\right]\right]\Phi_i(\vec{r}) = \varepsilon_i\Phi_i(\vec{r})$$

These equations are solved in this work using FP-LAPW method implemented in WIEN2k package.

For the calculations of structural and electronic properties of GaAs we used Muffin Tin approximation (MTA). The Muffin Tin radii R_{MT} values for Ga and As were set to 2.09 a.u. To perform calculations in this scheme division of the unit cell is done into muffin tin (MT) sphere and interstitial region. Potential, inside MT sphere is assumed to be spherically symmetric, while constant out of it. In our calculations for well convergence of energy, we used 35 k points in the irreducible wedge of the Brillion zone, $R_{MT} \times K_{max} = 8$, and a larger value of Gmax =14.

RESULTS AND DISCUSSIONS

Simulated unit cell structure of GaAs has been shown in Fig. 1. Total energy calculations were performed as a function of volume which can be seen in fig.2. We fitted the obtained data into Birch Murnaghan equation of state in other to obtain equilibrium values of structural parameters.

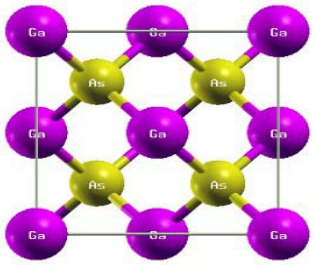

FIGURE 1. Unit cell structure of GaAs.

Our calculations for lattice constants, bulk modulus, its pressure derivative, and total energies are listed in Table 1 with different exchange correlation for comparison along with other computational and experimental results. From the table it can be seen though our results with all three exchange-correlation functional are close to the experiment and in good agreement with previous theoretical investigations, calculated value of lattice constant 'a' with GGA-WC is only 0.2% larger from experimental value which point out it as a good approach of exchange correlation energy functional in order to calculate the lattice parameters. However GGA-PBE gives slightly higher while the LDA produce slightly small value of 'a' in comparison with experiment. This observed discrepancy of LDA and PBE-GGA of our results as compared to that of experimental values is a well established fact. While for bulk moduli the LDA results are closer to experimental as compared to GGA-PBE and GGA-WC.

TABLE 1.The calculated data is compared to the experimental and other theoretical data available in the literature.

GaAs	Present Work		Experimental Work	Other Theoretical Work	
lattice constant, a(A^0)	GGA-PBE	5.749	**5.654**[5]	FP-LDA	5.608[4]
	GGA W-C	5.665	**5.653**[6]	FP-GGA	5.748[4]
	LDA	5.607		PP-LDA	5.530[7]
				PP-GGA	5.700[8]
				FP-LDA	5.651[9]
				FP-LDA	5.508[10]
				FP-LDA	5.649[11]
				FP-LDA	5.592[12]
				FP-GGA	5.726[12]
				HF	5.755[13]
				HF	5.760[14]
Volume V_0 (a.u)^3	GGA-PBE	320.652		FP-LDA	297.606[4]
	GGA W-C	306.749		FP-GGA	320.309[4]
	LDA	297.380			
Bulk Modulus B_0 (GPa)	GGA-PBE	60.84	**77.0**[17]	FP-LDA	75.2[4]
	GGA W-C	68.10	**76.0**[16]	FP-GGA	60.8[4]
	LDA	72.40		PP-LDA	75.7[7]
				PP-GGA	65.0[8]
				FP-LDA	63.0[9]
				FP-LDA	77.1[10]
				FP-LDA	74.2[11]
				FP-LDA	81.1[12]
				FP-GGA	68.0[12]
				HF	87.0[13]
				HF	77.0[14]
Pressure derivative B’	GGA-PBE	4.256	**4.487**[17]	FP-LDA	4.814[4]
	GGA W-C	4.394		FP-GGA	4.800[4]
	LDA	4.539		PP-LDA	4.487[7]
				FP-LDA	4.800[11]
				FP-LDA	4.460[12]
				FP-LDA	4.450[12]
Total Energy E_0 (eV)	GGA-PBE	-8410.487			
	GGA W-C	-8408.593			
	LDA	-8398.848			
Energy Band Gap E_g (eV)	GGA-PBE	0.329	**1.42**[18]	FP-LDA	0.28[7]
	GGA-WC	0.206		FP-GGA	0.51[7]
	LDA	0.099		FP-GGA-EV	1.03[4]
	LDA-MBJ	1.613		FP-LDA	0.23[9]
				FP-LDA	0.18[13]
				FP-LDA	0.09[14]
				FP-GGA-EV	0.97[15]
				FP-LDA	0.32[8]
				FP-LDA	0.49[8]

Calculated band structure of GaAs with GGA-PBE, GGA-WC, LDA and LDA+MBJ is presented in Fig. 3.

Since the calculated DOS with different approaches of exchange correlation Potential is similar. Thus we are explaining the DOS calculated with LDA+MBJ approach. Partial DOS of GaAs

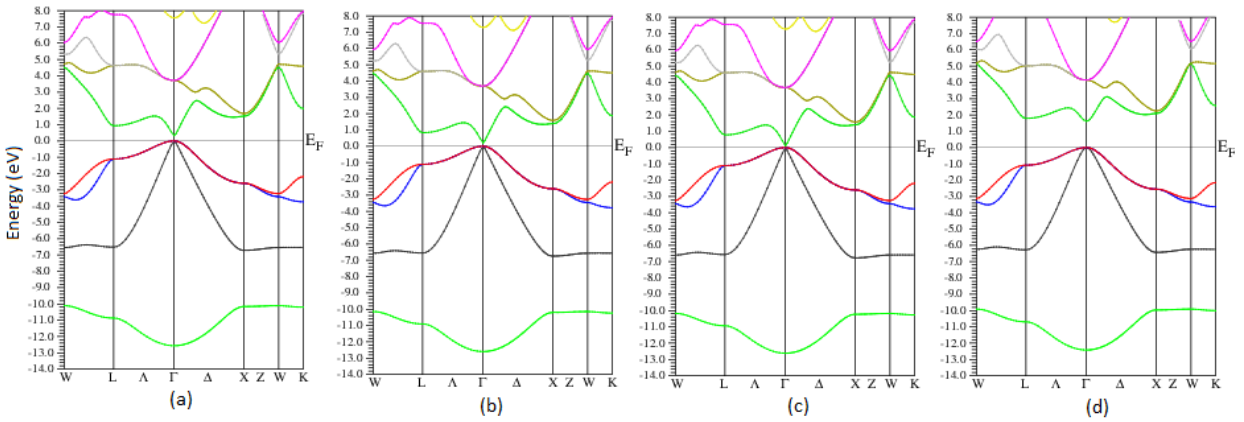

FIGURE 3. The electronic structure of GaAs with various exchange correlation potential have been shown. (a),(b),(c) and (d) shows the calculated band structure with GGA-PBE, GGA-WC, LDA and LDA +MBJ.

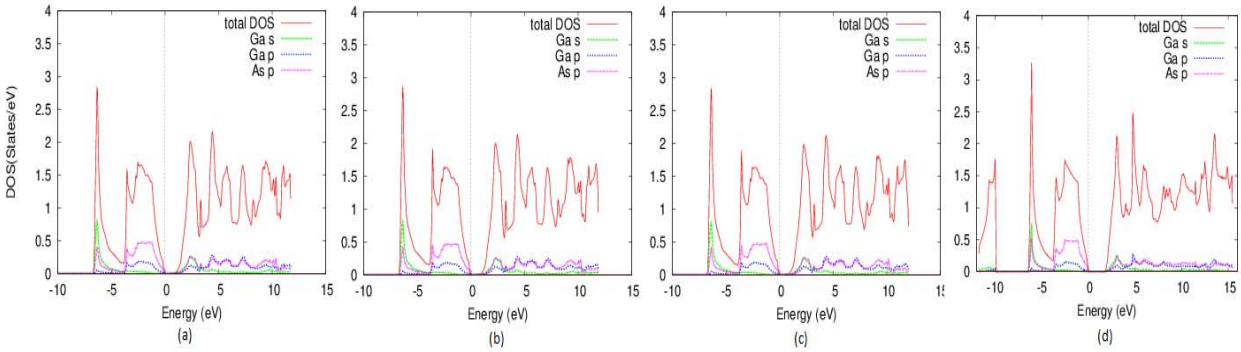

FIGURE 4. The density of states of GaAs with various exchange correlation potential have been shown. (a),(b),(c) and (d) shows the calculated DOS with GGA-PBE, GGA-WC, LDA and LDA-MBJ.

The knowledge of band structure energies is essential for the determination of electronic and optical properties of materials. Fig. 3 shows that LDA +MBJ exhibit a wider band gap followed by GGA-PBE, GGA-WC and LDA. Also the Fig.3 shows that valence band maximum and conduction band minimum lie at the same Γ-point that shows direct band gap behavior of GaAs. From Table.1 it is clear that band gap value calculated with MBJ +LDA approach is in better agreement to experimental value when it is compared to GGA-PBE, LDA and GGA-WC. Total and partial density of states (DOS) of GaAs with GGA-PBE, GGA-WC, LDA and LDA+MBJ exchange correlation potentials have also been shown in Fig. 4.

display a wide and broadened peak at energy range -12.4 to -9.9 eV originated from As-4s state. From -6.2 eV to -4 eV the states are mainly from Ga-4s and As-4p along with a weak contribution As-4s states. From -4 eV to the Fermi level (E_f) the states are mainly hybridization s and p electrons of Ga and p electrons of As. Whereas conduction band minimum is mainly formed by mixed states of Ga-4s and Ga-4p, As-4s and As-4p states.

CONCLUSION

In this work we carried out calculations for structural and electronic properties of GaAs with local density approximation (LDA), Perdew-Burke-

Ernzerhof parameterized generalized gradient approximation (PBE-GGA), Wu-Cohen parameterized GGA(WC-GGA) and modified Becke-Johnson exchange potential (MBJ) + LDA implemented in WIEN2k code. Our result for lattice constant with WC-GGA nicely agrees to experiment with a minor error of 0.2% experimental value. Although our calculated band gap value with LDA, PBE-GGA, WC-GGA is underestimated, with MBJ + LDA it is more accurate and is in good agreement to experimental energy gap value.

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