Calculations of Ground State Cohesive Properties of GaAs Crystalline Structure

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Abstract

We study different phases of GaAs crystalline structure andthe ground state cohesive properties of the most-stable structure of GaAs are computed within generalized gradient approximations GGA and the local-density approximation LDA of the density-functional theory using FHI-aims code.Among the phases of GaAs crystal studied zincblende structure is found to be the most-stable structure of GaAs crystal. The computed ground state properties such as lattice constant, cohesive energy and bulk modulus are 5.62 A^0, -5.27 eV and 71.9 GPa respectivelyand are found to be in agreement with experimentally found values within reasonable percentage errors.

1.0   Introduction

Gallium arsenide (GaAs) is among the most technologically important and the most studied compound semiconductor materials. It is used in the manufacture of devices such as microwave frequency integrated circuits, monolithic microwave integrated circuits, infraredlight-emitting diodes, laser diodes, solar cells and optical windows[1,2].

The diamond lattice structure is very common in semiconductor materials, such as Si, Ge. GaAs and GaP has a zincblende lattice structure which is similar to the diamond lattice structure. The diamond and zincblende structures are similar except that in diamond structure there is only one type of atom(see Fig.1a.) whereas in zincblende there are two types of atoms. In the GaAs unit cell there are four Ga-atoms and the rest are As-atoms(see Fig.1.b.).

Calculation of the bulk ground state properties, such as lattice constants, bulk modulus, cohesive energy, and atomic positions, play an important role in the physics of condensed matter [3,4].Bulk calculations help us to understand, characterize, and predict mechanical properties of materials in surroundings, under extreme conditions[5].

The cohesive energy of crystalline solid structure is defined as the energy that must be added to the crystal to separate its components into neutral free atoms at rest at infinite separation, with the same electronic configuration[6]. The term lattice energy is used in discussion of ionic crystals and is defined as the energy that must be added to the crystal to separate its component ions into free ions at rest at infinite separation.
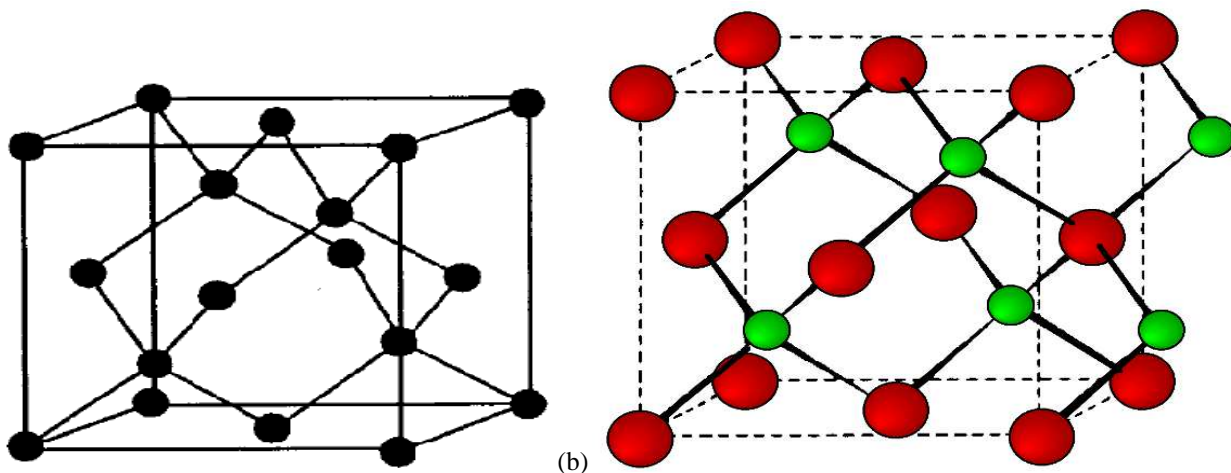

(b)

Fig 1. Unit cell structure of (a) Diamond cubic cell and (b) zincblende (GaAs) lattice. Ga atoms are shown small, As atoms shown large, and the dashed lines show the unit cell.

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Density-functional theory is one of the most popular and successful quantum mechanical approaches to matter. It is nowadays routinely applied for calculating, e.g., the binding energy of molecules and the band structure of solids in Physics[7,8,9].

Density Functional Theory (DFT) is a ground-state theory in which the emphasis is on the charge density as the relevant physical quantity[10,11,12]. DFT has proved to be highly successful in describing structural and electronic properties in a vast class of materials, ranging from atoms and molecules to simple crystals to complex extended systems (including gasses and liquids). Furthermore DFT is computationally very simple. For these reasons DFT has become a common tool in first-principles calculations aimed at describing or even predicting properties of molecular and condensed matter systems [7, 10, 12, 13].

Modern first principles calculations for extended systems of metals, semiconductors, and insulators are often based on density functional theory. The theory was placed on a rigorous foundation by Hohenberg and Kohnwho showed that the properties of a system of electrons and nuclei, in the ground state, are determined uniquely by the electronic charge density[8, 14]. The total energy of the system is therefore a unique functional of this charge density. Furthermore, they showed that the functional, whatever it is, is minimized by the true electronic charge density. The next important step was taken by Kohn and Sham, who showed that the problem of N interacting electrons could be mapped exactly onto N independent electrons, each moving in an effective single particle potential which emulates the interactions with all other electrons[9, 13]. In this way density functional theory has reformulated the many interacting electron problem, in which the central quantity is the many electron wave function, in terms of non-interacting electrons moving in an effective potential that describes all the electron interactions and in which the central quantity is the electronic density. The single particle equations are

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{eff}(r)\right)\psi_i(r) = \epsilon_i\psi_i(r) \qquad (1)$$

whereV_{eff} is the local effective mean potential, which depends on electron density only,ψ_i and ϵ_i are the single particle wave function and eigenvalue respectively. The density of the non-interacting system given by

$$n(r) = \sum_i^N |\psi_i(r)|^2 \qquad (2)$$

will reproduce the exact density of the interacting system. Again the energy of the non-interacting system will reproduce the exact ground state energy of the interacting system. The existence of the this potential is interesting but the use of density functional theory depends on finding approximation for V_{eff}that can be used in practical computations[9]. Typically, $V_{eff}$is expanded into:

$$V_{eff} = V_H + V_{e-nuc} + V_{xc} \qquad (3)$$

Where V_H is the Hartree potential due to electron-electron interaction,V_{e-nuc} is potential due to electron-nuclear interactionand the remaining term is the exchange-correlation potential, V_{xc}.

A great variety of different approximations to V_{XC} have been developed. Those approximations are (i) Local Density Approximation, LDA, (ii) Generalized Gradient Approximation, GGA and (iii) Hybrid Approximation[12, 13]. For many years the local density approximation (LDA) has been used. In the LDA the exchange correlation energy density at a point in space is taken to be that of the homogeneous electron gas with the local electron density,$\varepsilon_{xc}(n)$[8, 12, 15, 16].Thus the total exchange correlation energy functional is approximated as,

$$E_{xc}^{LDA} = \int n(\vec{r})\,\varepsilon_{xc}(n(\vec{r}))d\vec{r} \qquad (4)$$

from which the potential is obtained as,

$$V_{xc} = \frac{\delta E_{xc}}{\delta n} \qquad (5)$$

For many years properties such as structure, vibrational frequencies, elastic-moduli and phase stability are described very reliably for many systems. However, in computing energy differences between rather different structures the LDA can have significant errors[17]. For instance, the binding energy of many systems is overestimated and energy barriers in diffusion or chemical reactions may be too small or absent. Currently, effective potentials that depend both on the local density and the magnitude of its local gradient – so called, generalized gradient functionalare widely used [14]. The GGA approach in its various forms goes some way to correcting the problems seen in LDA calculations.

Solids are stable structures, and therefore there exist interactions holding atoms in a crystal together. For example a crystal of sodium chloride is more stable than a collection of free Na and Cl atoms. This implies that the Na and Cl atoms attract each other, i.e. there exist an attractive interatomic force, which holds the atoms together[18]. This also implies that the energy of the crystal is lower than the energy of the free atoms. The amount of energy which is required to pull the crystal apart into a set of free atoms is called the cohesive energy of the crystal.

Cohesive energy = energy of free atoms – crystal energy

Magnitude of the cohesive energy varies for different solids from 1 to 10 eV/atom, except inert gases in which the cohesive energy is of the order of 0.1eV/atom[19]. The cohesive energy controls the melting temperature .

Calculation of the bulk ground state properties, such as lattice constants, bulk modulus, cohesive energy, and atomic positions, play an important role in the physics of condensed matter[4], bulk calculations help us to understand, characterize, and predict mechanical properties of materials in surroundings, under extreme conditions.

2.0 Methodology

2.0 FHI-aims Code

FHI-aims("FritzHaberInstituteabinitiomolecularsimulations")isacomputerprogram package for computational materials science based on quantum-mechanical first principles. Themainproductionmethodisdensityfunctionaltheory(DFT) to compute the total energy and derived quantities of molecular or solid condensed matterinitselectronicgroundstate. Inaddition,FHI-aimsallowstodescribeelectronic single-quasiparticleexcitationsinmoleculesusingdifferentself-energyformalisms,andwave-functionbasedmoleculartotalenergycalculationbasedonHartree-Fockandmany-bodyperturbationtheory[20].

The focus here is on density-functional theory (DFT) in the local and semi-local (generalized gradient) approximations, but an extension to hybrid functionals, Hartree–Fock theory, and MP2/*GW* electron self-energies for total energies and excited states is possible within the same underlying algorithms. An all-electron/full-potential treatment that is both computationally efficient and accurate is achieved for periodic and cluster geometries on equal footing, including relaxation and *ab initio* molecular dynamics[21]. The construction of transferable, hierarchical basis sets is demonstrated, allowing the calculation to range from qualitative tight-binding like accuracy to meV-level total energy convergence with the basis set. Together with a scalar-relativistic treatment, the basis sets provide access to all elements from light to heavy. Both low-communication parallelization of all real-space grid based algorithms and a ScaLapack-based, customized handling of the linear algebra for all matrix operations are possible, guaranteeing efficient scaling (CPU time and memory) up to massively parallel computer systems with thousands of CPUs[21].

To compute the ground state cohesive properties of .GaAs crystal structure, we first calculate the ground state total energies of the most-stable structure of GaAs as a function of its lattice constants. The energies are then converted to the cohesive energies as a function of its molecular volumes using the equations[5, 22].

$$E_{coh} = -\frac{E_{bulk} - NE_{atom}}{N} = -\left[\frac{E_{bulk}}{N} - E_{atom}\right] \qquad (6)$$

The equilibrium quantities such as the lattice constant a_0, the cohesive energy E_{coh}, molecular volume, V_0, the bulk modulus B_0 and its derivative with respect to pressure B'_0 can be obtained by use a thermodynamically motivated and more accurate fitting function, the Birch-Murnaghan equation of states[22] given by

$$E(V) = E_0 + \frac{B_0 V}{B'_0}\left[\frac{(V_0/V)^{B'_0}}{B'_0 - 1} + 1\right] - \frac{B_0 V_0}{B'_0 - 1} \qquad (7)$$

2.1 General Computational Requirement

All calculations are carried out using fhi-aims code upgrade 5 (released on 17th July, 2011; version 071711_5). It only works on any Linux based operating system. Computations can only be carried out after building an executable binary file. Since the fhi-aims package is distributed in a source code form,

a. A working Linux-based operating system (Ubuntu 11.10 in this case)

b. A working FORTRAN 95 (or later) compiler. In this case we use x86 type computer and therefore intel's ifort compiler (specifically Composerxe 2011.6.233) was installed for this work.

c. A compiled version of lapack library, and a library providing optimized linier algebra subroutines (BLAS). Standard libraries such as Intel's mkl orIBM's essl provide both lapack and BLAS support. Intel's composerxe 2011.6.233 comes with mkl.

All necessary adjustment are made for building the executable binary file for running the code and the executable program was successfully build.

FHI-aims requires two input files: (1). **control.in:-** which contains all runtime-specific informations and (2). **geometry.in**:- which contains information directly related to the atomic structure for a given calculation. The two input files must be places in the same directly from where the FHI-aims binary file is invoked at the terminal.

2.2 Construction of the Input Files and Running the FHI-aims Code

Our first step towards studying periodic systems with FHI-aims is to construct periodic geometries in the FHI-aims geometry input format (**geometry.in**). Next, we set basic parameters in **control.in** for periodic calculations. Finally, we compare total energies of different GaAs bulk geometries.

A **geometry.in** files for the GaAs bcc and zincblende structures were constructed using the experimental lattice constants a of 5.3 Å for bcc and 5.6 Å for zincblende.

In setting up the **geometry.in** file of a periodic structure in FHI-aims all three lattice vectors as well as the atomic positions in the unit cell are specified. The lattice vectors are specified by thekeyword **lattice_vector**. For example, the GaAs bcc structure with a lattice constant ain Å is specified in the following format:

```
lattice_vector          -a/2      a/2      a/2
lattice_vector           a/2     -a/2      a/2
lattice_vector           a/2      a/2     -a/2
atom    0.0     0.0      0.0  Ga
atom    a/4     a/4      a/4  As
```
Similarly the GaAs zincblende structure with a lattice constant a in Å is specified as
```
lattice_vector          -0.0      a/2      a/2
lattice_vector           a/2      0.0      a/2
lattice_vector           a/2      a/2      0.0
atom    0.0     0.0      0.0  Ga
atom    a/4     a/4      a/4  As
```
A **control.in** input files for GaAs was created with the following settings.
```
# Physical settings
xc          pw - lda
spin      none
relativistic atomic_zora scalar
# SCF settings
charge_mix_param        0.2
n_max_pulay             8
sc_accuracy_eev  1E-2
sc_accuracy_etot 1E-5
sc_accuracy_rho  1E-4
sc_iter_limit            40
# k - grid settings
k_grid  3  3  3
```
The above settings basically define pw-lda as the exchange-corralation approximation and the self-consistance covergence criteria. In addition to the above parameters, the default "light" species settings for Ga and As as supplied with the code were also incooparated in to the control.in file.

A bash script named **run.sh** was created to calculate total energies of the different phases of GaAs as a function of lattice constant a. For this, seven different values of a in steps 0.1 Å around the lattice constants given above was used for each structure.

Note that the grid factors refer to the reciprocal lattice vectors corresponding to the real-space lattice vectors in **geometry.in**. If there are inequivalent lattice vectors, their order in **geometry.in** determines the ordering of reciprocal lattice vectors in the code.

The total energy per atomfor each structure is plotted as a function of the lattice constant using a ploting software ORIGIN. The most stable structure was determined from the plot.

The above procedure was repeated using GGA as the exchange-correlation. Also all calculations done for zincblende were repeated for GaAs bcc structure.

2.3   Energy Convergence Tests
Having zincblende phase found to be the moststable structureof GaAs, we nextinvestigate total energy convergence for zincblende GaAs with respect to the k-grid and basis set.

2.3.1   k-grid convergence test
The total energies for zincblende GaAs was calculated as a function of the lattice constant for k-grids of 8×8×8, 10x10x10, 12×12×12, and 16×16×16 using the minimal+spd basis set. The same computational settings and the same lattice constants as in the previous calculations of section **2.2** was used. Graphs of the total energy and the computational time against lattice constant were plotted . The results of 3×3×3 from previous runs was added. From the plots the k-gridproducing the minimal energy for GaAs zincblende was found.

2.3.2   Convergence with basis set size
The total energies for zinblende as a function of the lattice constant for the minimal and the tier1 basis sets are calculated. The same lattice constants and computational settings as in **2.2** together with the 10×10×10 k-grid are used. Again, similar plotsas in 2.3.1 were made but for the minimal and tier1 basis set calculations. The results for the minimal+spd basis set obtained in 2.3.1 was also added to the results. Again from the plot the basis set for which the GaAs zincblende structure gives the minimal energy and minimal convergence time is determined.

2.4   Phase Stability and Cohesive Properties
After finding "converged" computational settings, we now revisit the phase stability of bulk GaAs.Note that in practice check convergence must be achieved first in order to avoid false conclusions. We will now compute the basic cohesive properties and study the pressure dependence of phase stability.

2.4.1 Recalculation of E(*a*) curves

The total energies of bcc GaAs as a function of lattice constant *a* are calculated. The settings from section **2.3** (k-grid of $10\times10\times10$, minimal+spd basis) and the same lattice constants as in section **2.1** were used. The results obtained and that of zincblende GaAs obtained in section 2.3 were plotted as in section **2.2** and the plots were analyzed to arcertain the most stable phase of GaAs crystall.

2.4.2 Calculations of Cohesive energies and atomic volumes

The total energy of a free atomfor GaAs unit cell zincbladeis calculated as follows: For the single atom energy, special care has to be taken. First, the free atom is of course spin polarized and we use **"spin collinear"** instead of "spin none" as well as properly initialize the magnetization with **"default_initial_moment hund"**. Second, we use a more converged basis. In particular, we use all basis functions up to "tier 3", the cutting potential was increase to **"cut_pot 8. 3. 1."**, and basis dependent confining potentials was turned off with **"basis_dep_cutoff 0"**

The cohesive energy (Ecoh) of a crystal is the energy per atom needed to separate it into its constituent atoms. E_{coh} is defined as

$$E_{coh} = -\frac{E_{bulk} - NE_{atom}}{N} = -\left[\frac{E_{bulk}}{N} - E_{atom}\right]$$

where E_{bulk} is the bulk total energy per unit cell and *N* the number of atoms in the unit cell. E_{atom} is the energy of the isolated atom calculated above.

In order to compare the pressure dependence of phase stabilities we need to express the lattice constant behavior of all phases on equal footing. One possibility to do so is to express the lattice constant in terms of the volume per atom. This atomic volume can be calculated quite easily from the lattice constant *a*. The simple cubic (super-)cell has the volume $V_{sc} = a^3$. This number has to be divided by the number of atoms *N*sc in this cell $V_{atom} = a^3/N_{sc}$. Note that there are two, and eight atoms in the simple cubic supercell in the case of the *bcc*, and the zincblende structure, respectively.

A file *energy.dat* containing the lattice constants and total energies per atom was converted to a file *cohesive.dat* containing atomic volumes V_{atom} and (negative) cohesive energies $-E_{coh}$ by the use of the script *convert-coh.awk* which is provided in the code.

2.4.3 Calculation of cohesive properties at equilibrium.

An important equilibrium quantity we can calculate from our data is the equilibrium lattice constant a_0. In principle, this can be done with a quadratic ansatz for *E*(*a*) or *E*(*V*). Here we will use a thermodynamically motivated and more accurate fitting function, the Birch-Murnaghan equation of states[22]. The energy per atom ($E = -E_{coh}$) is expressed as a function of the atomic volume ($V = V_{atom}$) as in equation (7).

The cohesive energy data for the zincblende phase of GaAs calculated above was fitted to the Birch-Murnaghan equation of states using the program **murn.py**. The lattice constant *a*, the bulk modulus B_0, and the cohesive energy per atom E_{coh} at equilibrium are determined. The calculated cohesive properties in this work are compared with the experimental values and those determined in other theoretical works.

2.5 Convergence Test and Calculations of Cohesive Properties Using fine-tuned Lattice constants.

From the plots of section **2.2** the lattice constant that give the minimum total energy was determined for both bcc and zincblende GaAs crystal structure up to four decimal places of accuracy. The same was repeated for the k-grids of 8x8x8, 10x10x10, 12x12x12 and 16x16x16 of zincblende structure. The FHI-aims was run to calculate the total energies for, seven different values of *a* in steps 0.0001 Å around the lattice constants found above for each structure. The resultant k-grid was used to carried-out the basis convergence test as in section **2.2**. The result obtained for the basis convergence was used to calculate the cohesive properties such asV_0, the equilibrium molecular volume, E_0, the molecular energy,the equilibrium lattice constant a_0, the bulk modulus, B_0 and B'_0 derivative with respect to pressure of bulk modulus as in section **2.3.2.**

3.0 Results

3.0 Introduction

The the output files of the computationswere use to deduce the tables of lattice constants against the total energies and graphs were plotted to obtain the optimized parameters for GaAs structures within both LDA and GGA. The optimized parameters were then used to obtained the equilibrium ground state properties of GaAs.

3.1 Graphical Representation of Data

The following graphs summarize the output data obtained during the convergence test, and are used in obtaining the optimized values of the parameters investigated.
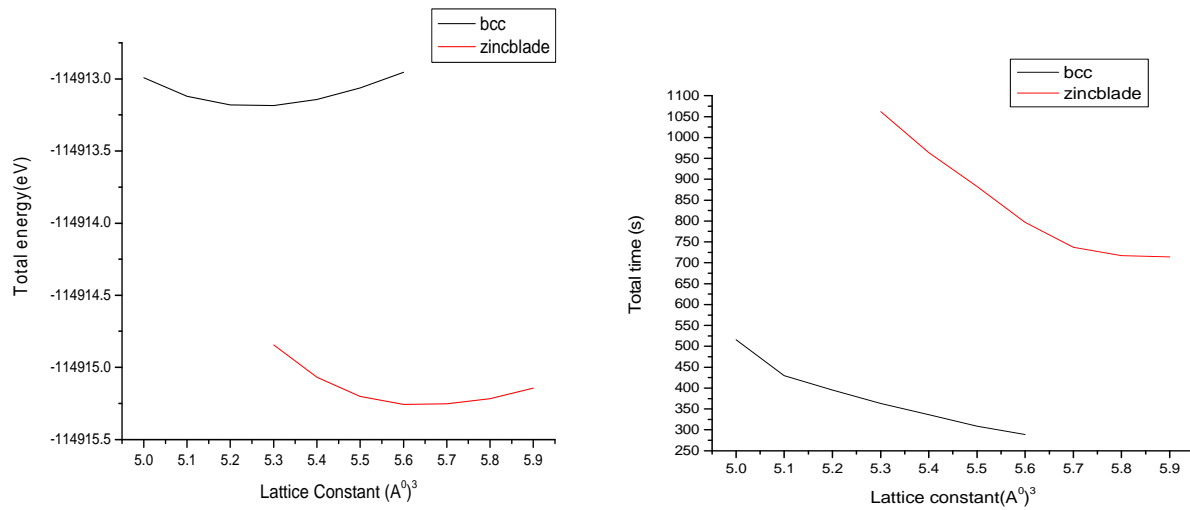
Fig.2. Plots of Total Energy (a) and Total time (b) against Lattice constant for bcc and zincblende GaAs structure within LDA xc functional
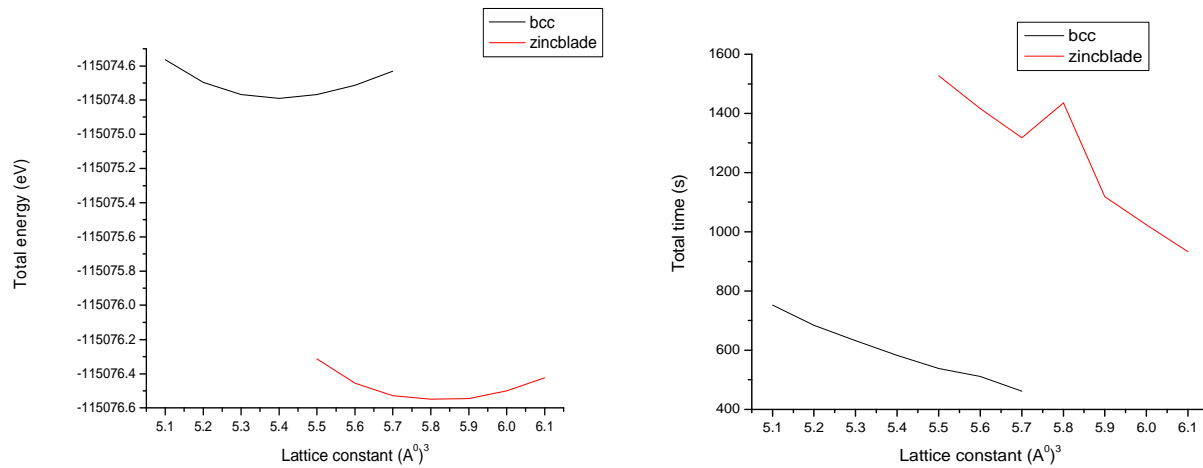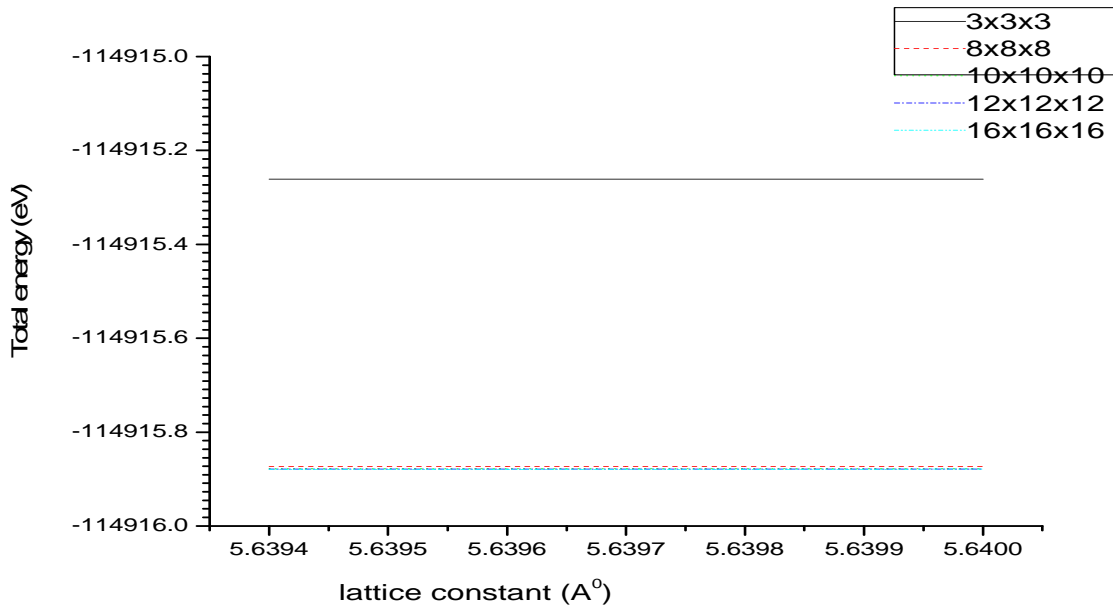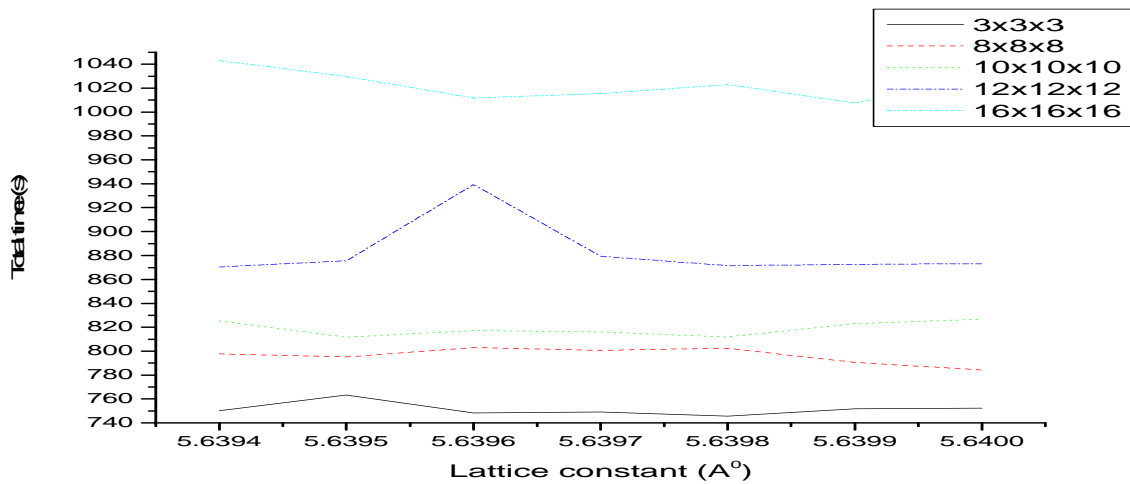

Fig 3 Plots of Total Energy (a) and Total time (b) against Lattice constant for bcc and zincblende GaAs structure within GGA xc functional
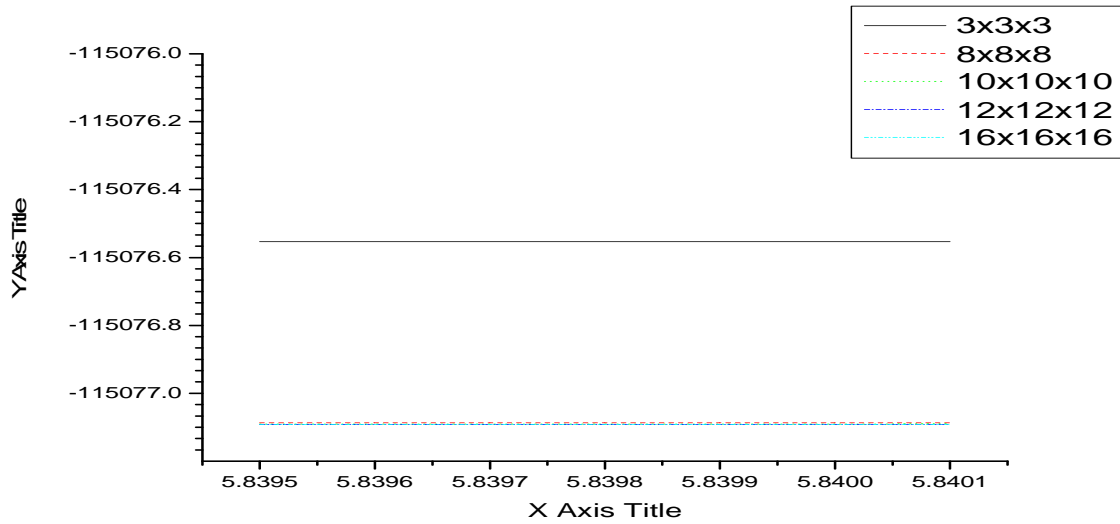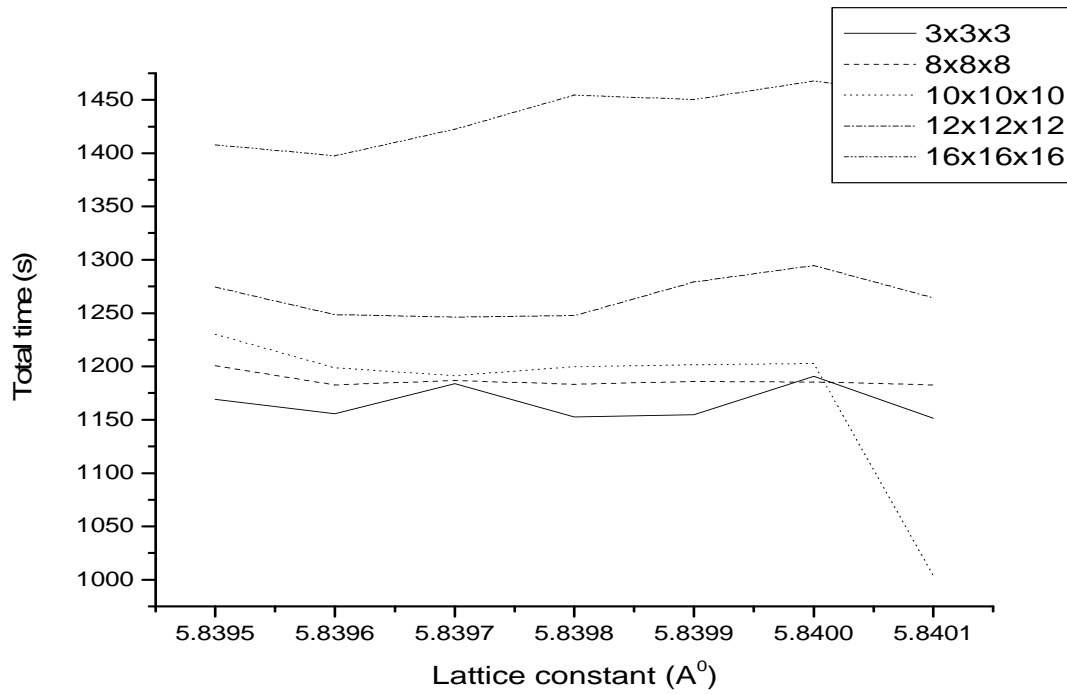
(a)

(b)

Fig .4. Plots of (a) Energies and (b) total times against lattice_constant up to 4 places of accuracy for various kgrids of GaAs zincblende structure within LDA.
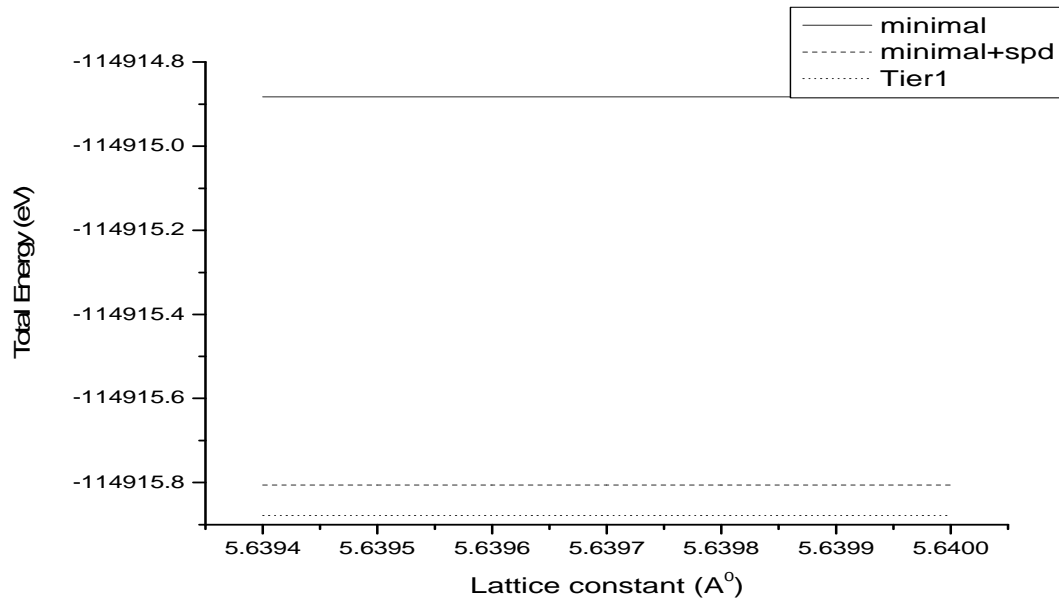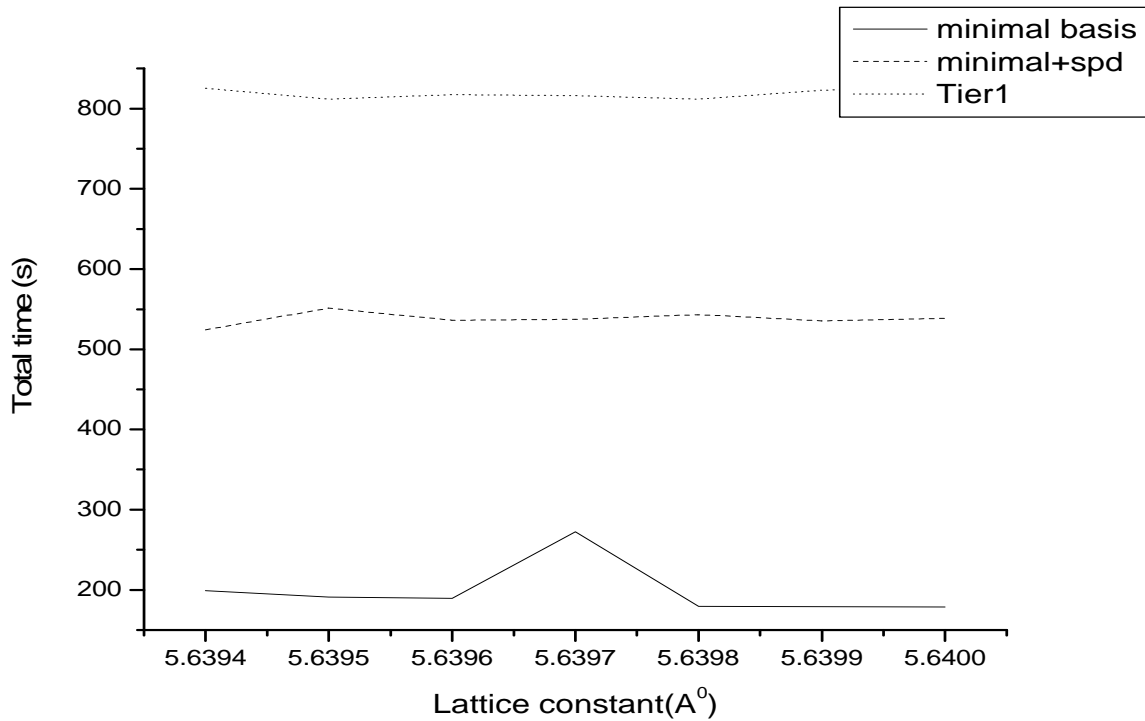
(a)

(b)

Fig.5. Plots of (a) total energies and (b) total time against lattice constants for various kgrids of GaAs zincblende crystal within GGA xc
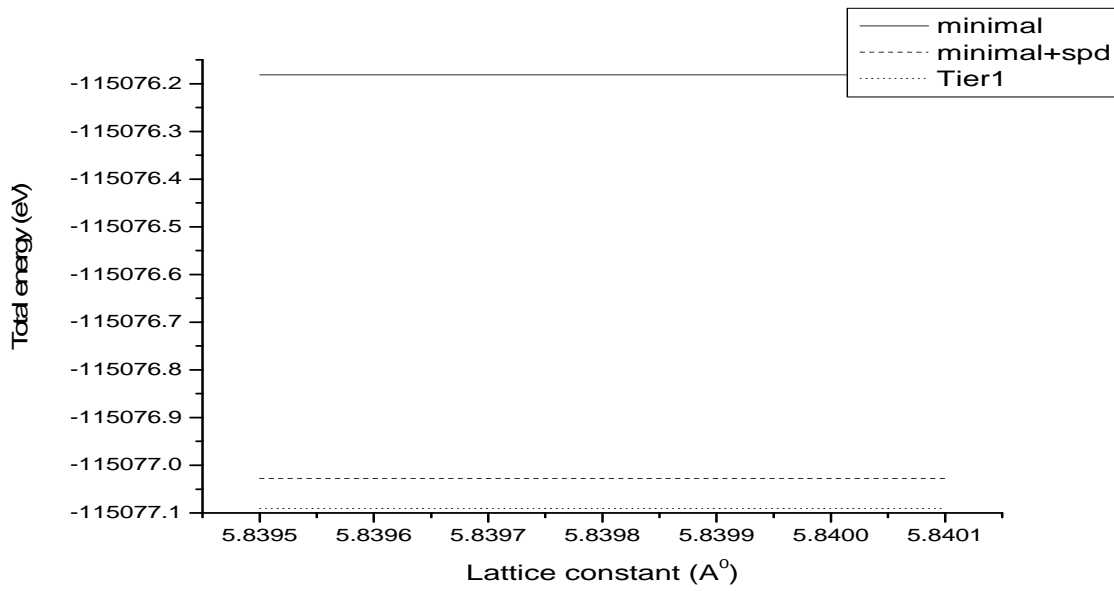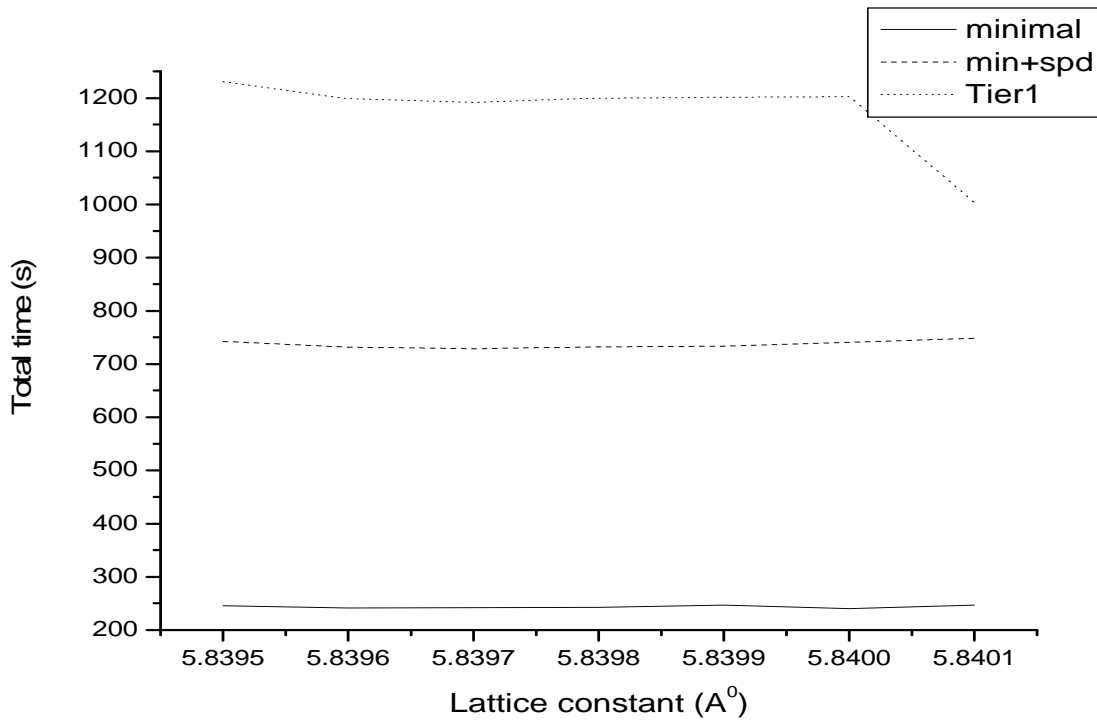
(a)

(b)

Fig..6. Plots of Plots of (a) total energies and (b) total time against lattice constant for three different basis of GaAs zincblende crystal within LDA

(a)

(b)

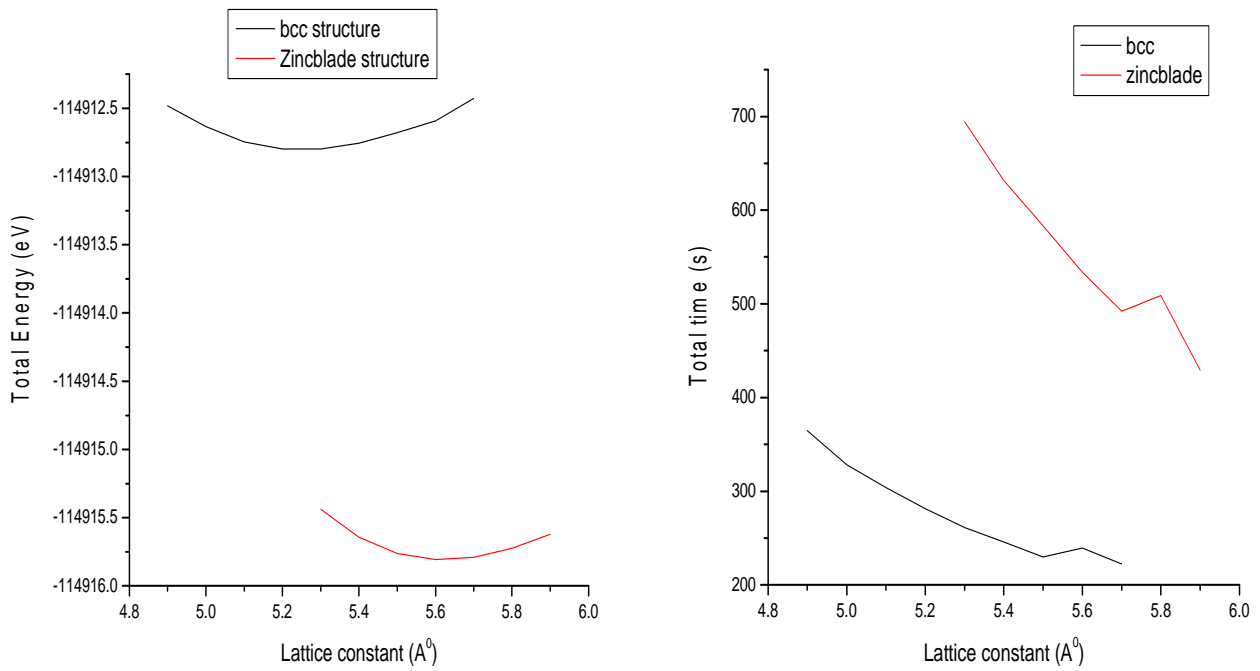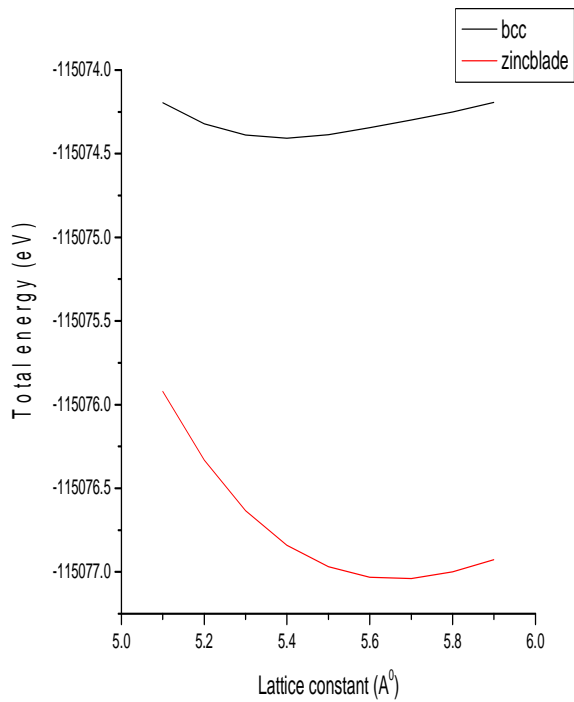Fig.7. Plots of Plots of (a) total energies and (b) total time against lattice constant for three different basis of GaAs zincblende crystal within GGA

(a)   (b

Fig.8 Plots of Total Energy (a) and Total time (b) against Lattice constant for bcc and zincblende GaAs structure within LDA xc functional with optimum kgrid of 10x10x10

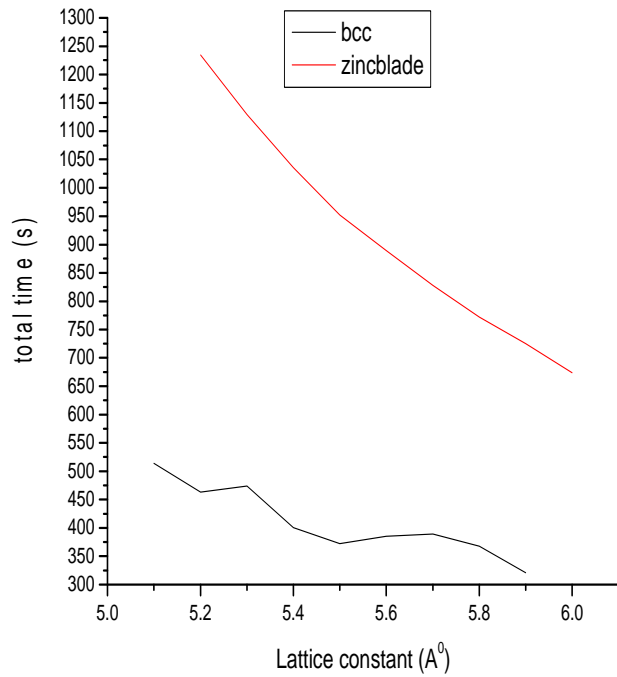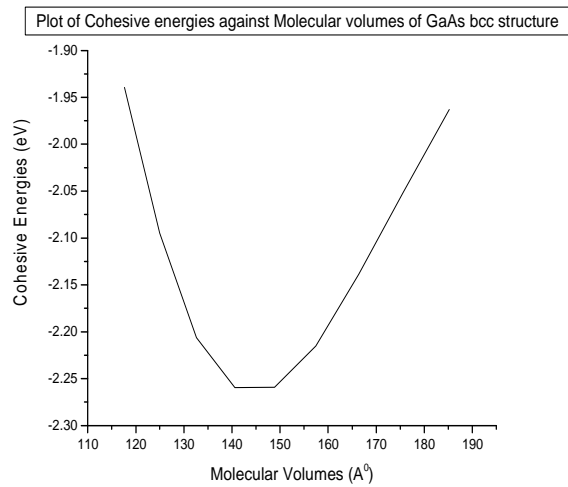(a)   (b)
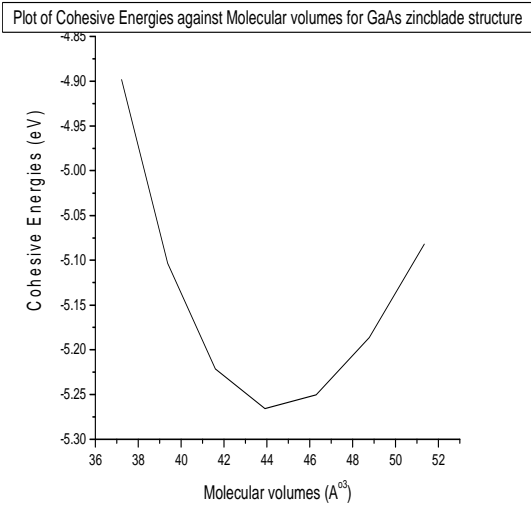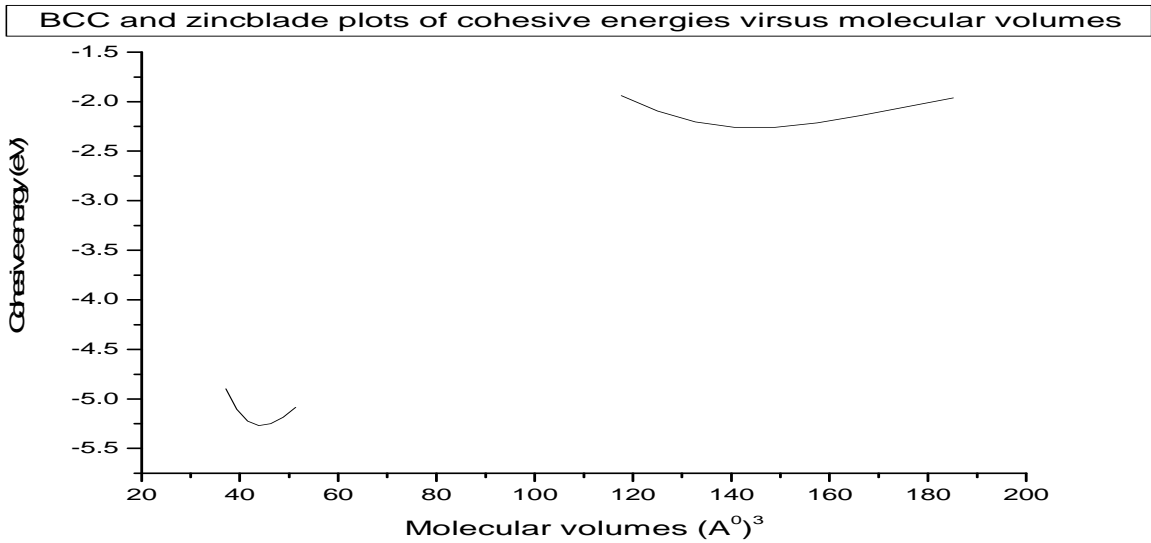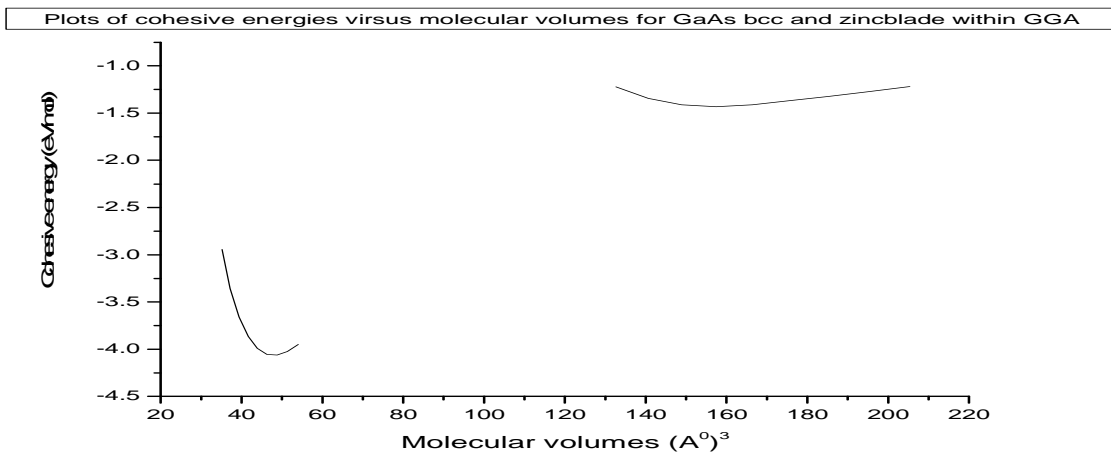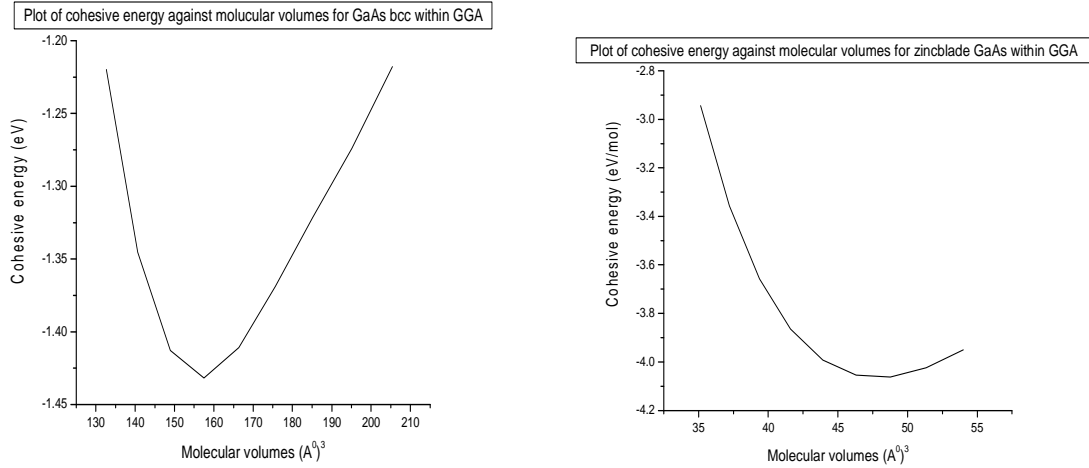

Fig 9 Plots of Total Energy (a) and Total time (b) against Lattice constant for bcc and zincblende GaAs structure within GGA xc functional

(a) (b)

Fig.10 Plots of cohesive energies virsus molecular volumes of bcc (top) and zincblende (down) structures of GaAs within LDA xc functional arrived at using coarse lattice-constant.

(a)   (b)

Fig.11 Plots of cohesive energies virsus molecular volumes of bcc (top) and zincblende (down) structures of GaAs within GGA xc functional arrived at using coarse lattice-constant.
Cohesive Energies(eV)
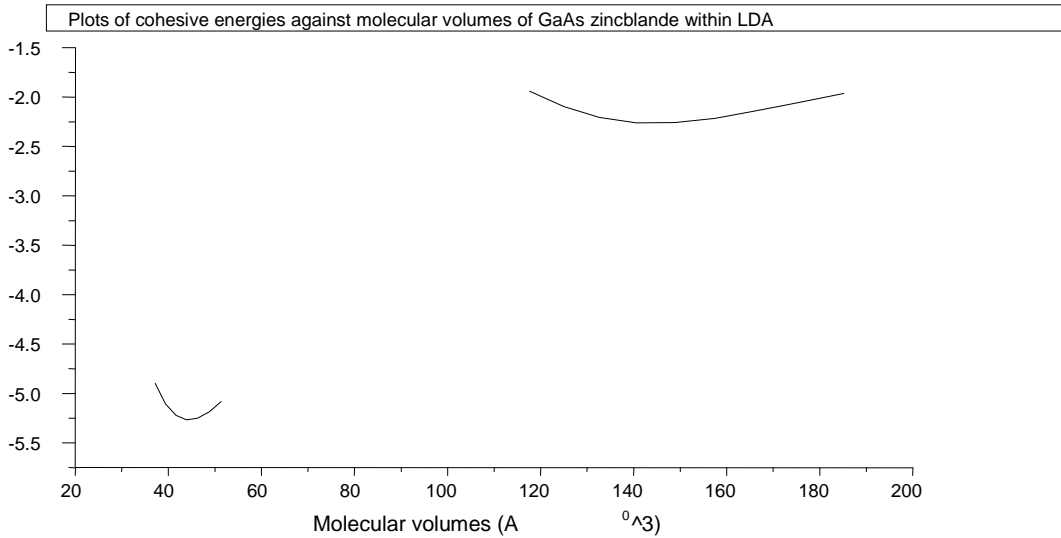
Fig.12 Plots of cohesive energies virsus molecular volumes of bcc (top) and zincblende (down) structures of GaAs within LDA xc functional arrived at using fine-tuned lattice-constant.

3.2 Tabular Representation Results

TABLE 1 List of minimum total energy and total time against lattice constant for determination of the most table phase of GaAs structure.

Phase	XC	Lattice-constant (A^0)	E_{min}(Ev)	Total time (s)
	LDA	5.3	- 114913.184762136	363.551
BCC	GGA	5.4	-115074.789260061	582.403
	LDA	5.6	-114915.256440864	797.029
ZINCBLENDE	GGA	5.8	-115076.549135505	1435.836

TABLE 2: COHESIVE PROPERTIES OF GaAs Zincblende crystal

Property	Present using GGA xc	Present using LDA xc	Experimental	Others
Lattice constant (Å)	5.7637368756 (fine-tuned) 5.766708068 (**coarse**)	5.621534223 (fine-tuned) 5.622386712 (**coarse**)	5.65 [2]	5.56 [23] 5.51 [24] 5.6542 [5]
Cohesive energy (eV/atom)	-4.06424031869 (fine-tuned) -4.06495344279 (**coarse**)	-5.26719923473 (fine-tuned) -5.26680811664 (**coarse**)	- 6.52 [25]	- 6.21, - 6.51 [23] , - 6.50 [5].
Bulk modulus B_0(GPa)	69.397467 (fine-tuned) 59.69468 (**coarse**)	71.907912 (fine-tuned) 71.627694 (**coarse**)	74.7 [2]	75.4, 60.4 [23] , 79.8 [5].
B'	3.45736985952 (fine-tuned) 4.18661338312 (**coarse**)	4.7089724784 (fine-tuned) 4.5768243934 (**coarse**)	3.36 [26]	3.686 [5].
E_{bulk}(eV)	-115077.040345860 at (5.76638 A) -115077.037268923 at (5.8 A)	-114915.806788347 at(5.6215) -114915.805441952 at (5.6 A)		

4.0   Discussion

From Fig.2and Fig.3 it could be seen that the total energy for zincblende phase of GaAs is much lower than that of body centred cubic phase calculated within both LDA and GGA. Thus, the zincblende phase seem to be more stable than the bcc phase and therefore is chosen to be the unit cell of interest in this work as in agreement with the experiment and other theoretical works.

From Fig. 4 and Fig. 5 you can see, the total energy calculated within LDA of the 3×3×3 calculation differs by about 0.62 eV from the most accurate (16×16×16) calculation. The larger part of this error is already fixedbythe8×8×8k-grid,which is still off by about 5.8 meV.The10×10×10 k-grid, on the other hand, is converged within about 1.5 meV. Lastly the 12x12x12 k-grid converges within only 0.43meV.

Looking at the computational times you see two general trends in FHI-aims. First, the times strongly decrease towards larger lattice constants. This is because there is less overlap between atoms and so less integrations are needed. The approach of FHI-aims is particularly efficient for"open"structures where the atoms occupy more space and thus have less neighbors. Second, increasing the number of*k*-points does not affect the calculation all times significantly up to comparablydense*k*-grids. A total energy calculation with a10×10×10 grid is not so much more expensive than a3×3×3 calculation. Only with even denser *k*-grids computational times increase note worthy.

Inconclusion,weshouldusea10×10×10 *k*-grid for zincblende GaAs is a good compromise of high accuracy and reasonable computational time.

From Fig 6. and Fig. 7. we can see that the minimal basis gives completely unphysical results; there is not even a energetic minimum within the calculated range of lattice constants. The minimal basis lacks the flexibility to give reasonable geometries. On the other hand, the binding curve does not change significantly from minimal+spdto the full tier1 basis set whereas the computational effort increases significantly by adding the *f* functions from minimal + spd to full tier1.

While the total energy difference of 70meV between minimal + spd and tier1 is still larger than what we were aiming for in the case of the *k*-grid, we can make use of the fact that the total energy is variational so that a large part of the basis set error actually cancels nicely in energy differences.

After finding "converged" computational settings, we now revisit the phase stability check of bulk GaAs as in section 3.1 before proceeding to calculate the basic cohesive properties avoid false conclusions. There resulting binding curves shown in Fig.8 clearly show that the experimentally observed zincblende structure of GaAs is most stable in LDA and GGA among the crystal structure studied in this work.

From the ground state cohesive properties of GaAs obtained as compared with the experimentally obtained values and other

theoretically computed results,the lattice-constants obtained is under estimated by about 0.03 A^0 for LDA and over estimated by about 0.11 A^0 for GGA calculation. The cohesive energy of GaAs computed in this work is over estimated by about 1.25 eV and 2.45 eV for LDA and GGA respectively. The bulk-modulus is under estimated for both LDA and GGA with error of 2.79 GPa and 5.30 GPa respectively.

Conclusion

The ground state cohesive properties such as the lattice constant, cohesive energy and bulk modulus of GaAs zincblende crystal within LDA and GGA were calculated. The values obtained are in agreement with the available theoretical and experimental values reported within some reasonable percentage errors.It could be concluded that thus, the lattice constant calculated for LDA and GGA are respectively -0.53% and +1.95% of the experimentally reported result. Also the Bulk modulus computed in this work for LDA and GGA are -3.7% and -7.1 % of the reported result.

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