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Determination and Optimization of Bulk Total Energy for Gallium-Arsenide (GaAs) Atom using FHI98MD Input Variables

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Result shows that the bulk total energies of - 8.6610957 were obtained for GaAs (LDA). This result of GaAs agrees well with the value -8.0691176 Rydberg/atom obtained 1999 by Stadelé et al and -8.364 Rydberg/atom obtained 2003 by Franziska Gizegoizewski.

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Abstract - The Optimization of bulk total energy Calculations have been performed using the Local Density approximation for the exchange-correlation functional of Perdew Wang, within density-functional theory (DFT) for Gallium-arsenide (GaAs) atom. The optimized values obtained were used to calculate the bulk total energy of Gallium-arsenide. These calculations were performed using the Density Functional Theory method which represents the most popular technique for examining a wide range of structural and electronic properties of semiconductors and its alloys. The DFT code FHI98MD was employed for this computation which contains seventy six input parameters / variables. Some of these variables were determined and calculated while seven parameters that determine electronic convergence were successfully optimized for Local Density Approximation (LDA).

Result shows that the bulk total energies of -8.6610957 were obtained for GaAs (LDA). This result of GaAs agrees well with the value -8.0691176 Rydberg/atom obtained 1999 by Stadele et al and -8.364 Rydberg/atom obtained 2003 by Franziska Gizegozewski.

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1. INTRODUCTION

This paper presents the results of first principles calculations of electronic structure by optimization of Bulk total energy for Gallium arsenide (GaAs). This is a compound of the elements gallium and arsenic. It is a III/V semiconductor, and is used in the manufacture of devices such as microwave frequency integrated circuits, monolithic microwave integrated circuits, infrared light-emitting diodes, laser diodes, solar cells and optical windows. (Moss and Ledwith 1987).

The intensive aspect of Hartree-Fock (HF) was circumvented when performing the first principle calculations considering the large system of atoms involved. Over the years, the use of density functional theory (DFT) as a solution towards solving these problems has been highly successful. In this method the electron density is treated as the fundamental variable (Hohenberg and Kohn, 1964; Kohn and Sham 1965) instead of the one-electron wavefunctions as in HF. Here the forces on the ions were calculated and the ion

positions with respect to the total energy were optimised. Fundamentally, we wish to solve the many-body Schrodinger equation for this specific set of atoms in a specific configuration, i.e.

$$H\Psi_i = E_i\Psi_i \quad (1)$$

where H is the many-body Hamiltonian, and Ψ is the many-body wave-function corresponding to the i^{th} state which has energy E_i . The term Ψ is a function of the electron spin and co-ordinates as well as the nuclear positions. The minimum value of E therefore represents the ground state of the system.

a) Theoretical Background

The approach used in this paper for the theory of electronic structure is that of DFT. In this approach, the electron density distribution $n(\mathbf{r})$ rather than the many electron wave-function plays a central role between the fully interacting many electron system (described by the schrodinger equation) and a fictitious system of non-interacting fermions. The fundamental proof of DFT is of the existence of a local, effective mean field potential, V_{eff} , which depends only on the electron density and for which, if one solves a set of single particle Schrodinger- like equations,

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

the density of the non-interacting system

$$n(\mathbf{r}) = \sum_{i=1}^N |\psi_i(\mathbf{r})|^2 \quad (3)$$

will reproduce the exact density of the fully interacting system. Moreover the energy of the non-interacting system reproduces the exact ground state energy of the interacting system. The existence of such a potential is fascinating but the utility of DFT is dependent on one finding a decent approximation for V_{eff} that can be used in practical simulations (Parr and Yang, 1989). Typically, V_{eff} is separated into an electron-nuclear (V_{en}), classical (Hartee) electron-electron interaction

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(V_H) and the remaining exchange-correlation potential (V_{xc}) ;

$$V_{eff} = V_{en} + V_H + V_{xc} \quad (4)$$

Where

$$V_H(r) = \int \frac{n(r')}{|r - r'|} dr' \quad (5)$$

a great variety of different approximations to V_{xc} have been developed.

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, $\epsilon_{xc}(n)$. Thus the total exchange correlation energy functional is approximated as

$$E_{xc}^{LDA} = \int n(r)\epsilon_{xc}(n(r))dr \quad (6)$$

from which the potential is obtained as,

$$V_{xc} = \frac{\delta E_{xc}}{\delta n} \quad (7)$$

The LDA has proven to be a remarkably fruitful approximation. However in computing energy differences between different structures, the LDA can have significant errors. 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 on local density approximation are widely used.

II. METHODOLOGY

In this work the DFT programmed used is fhi98md. It has start utility fhi98start, the input files constraints.ini, inp.mod, start. inp, fort.11 and fort.12 are all placed in a common folder. All 76 parameters / variables in the files inp.mod and start.inp are determined and calculated for this system of interest. The start utility is then run which produces three additional files: inp.ini, balsac and balsacclu.

The fhi98md program is then run which produces seventeen output files. These include the general output file fort.6; the file energy; restart files fort.71, fort.72, fort.73, fort.74, fort.80; control files stopfile, stopprogram and a host of other data files.

To optimize a given parameter, the program is run repeatedly changing the value of the parameter in each run. The total energy, Harris energy, internal energy at zero temperature (zero energy) and the number of iterations are recorded for each run. The values obtained are then used for:

- Convergence test by plotting parameter versus total energy;
- Accuracy test by plotting parameter versus absolute difference between total energy and Harris energy
- Speed test by plotting parameter versus number of iterations.

The optimal value of the parameter is then determined from the three plotted graphs.

For parameters that are logical in nature, the program is run with the parameter set to .true. and then re-run with the parameter set to .false.

We then used all optimal values obtained to calculate total energies for bulk Gallium-arsenide.

The optimal parameters used are as follows

Delt: step length of the electronic iterations

Gamma: damping parameter for the second order electronic minimization scheme

Ecut: plane wave energy cutoff (in Rydberg)

Ecuti: plane wave energy cutoff of the initial wave function

Ekt: temperature of the artificial Fermi smearing of the electrons

idyn: scheme for solving the equation of motion of the nuclei.

i_edyn: scheme to iterate the wave functions

tmetal: occupy electronic state

force_eps: convergence criteria for local and total forces

ion_damp: damping parameter

ion_fac: mass parameter/ mass of the nuclei

III. RESULTS AND DISCUSSIONS

The seven parameters that determine electronic convergence were optimized and several data were generated. The software "origin 5.0" was used to plot the graphs. These optimal values were then used to calculate the bulk total energy of Gallium-arsenide for Local Density Approximation.

a) Tables of Data

Table 1 : Delt Optimization for Gallium-arsenide LDA

Delt	Number of iterations	Total energy (E_T)	Harris energy (E_H)	ABS($E_T - E_H$)
10	27	-8.6076685	-8.6076687	0.0000002
20	16	-8.6076686	-8.6076688	0.0000002
30	15	-8.6076685	-8.6076686	0.0000001
40	18	-8.6076684	-8.6076686	0.0000002

50	25	-8.6076685	-8.6076686	0.0000001
60	52	-8.6076685	-8.6076687	0.0000002
70	99	-8.6076685	-8.6076687	0.0000002
80	99	-7.7738509	-7.7618081	0.0120428
90	99	-7.5559049	-7.6780074	0.1221025
100	99	-7.5032794	-7.625224	0.1219446

Table 2 : Gamma Optimization for Gallium-arsenide LDA

Gamma	Number of iterations	Total energy (E_T)	Harris energy (E_H)	ABS(E_T-E_H)
0.1	99	-7.5657386	-7.5719817	0.0062431
0.2	15	-8.6076685	-8.6076686	0.0000001
0.3	17	-8.6076685	-8.6076687	0.0000002
0.4	23	-8.6076685	-8.6076687	0.0000002
0.5	27	-8.6076686	-8.6076688	0.0000002
0.6	29	-8.6076685	-8.6076688	0.0000003
0.7	31	-8.6076685	-8.6076687	0.0000002
0.8	33	-8.6076685	-8.6076687	0.0000002
0.9	34	-8.6076686	-8.6076687	0.0000001
1	35	-8.6076686	-8.6076687	0.0000001

Table 3 : Ecut Optimization for Gallium-arsenide LDA

Ecuti	Number of iterations	Total energy (E_T)	Harris energy (E_H)	ABS(E_T-E_H)
1	20	-8.68585	-8.685852	0.0000003
2	17	-8.68585	-8.685852	0.0000001
3	14	-8.68585	-8.685852	0.0000002
4	13	-8.68585	-8.685852	0.0000000
5	13	-8.68585	-8.685852	0.0000000
6	13	-8.68585	-8.685852	0.0000000
7	13	-8.68585	-8.685852	0.0000000
8	13	-8.68585	-8.685852	0.0000000
9	13	-8.68585	-8.685852	0.0000000
10	13	-8.68585	-8.685852	0.0000000
11	13	-8.68585	-8.685852	0.0000000
12	13	-8.68585	-8.685852	-0.0000001
13	13	-8.68585	-8.685852	-0.0000001
14	13	-8.68585	-8.685852	0.0000000
15	13	-8.68585	-8.685852	-0.0000001
16	13	-8.68585	-8.685852	0.0000001

Table 4 : Ecuti Optimization for Gallium-arsenide LDA

Ecuti	Number of iterations	Total energy (E_T)	Harris energy (E_H)	ABS(E_T-E_H)
1	20	-8.68585	-8.685852	0.0000003
2	17	-8.68585	-8.685852	0.0000001
3	14	-8.68585	-8.685852	0.0000002
4	13	-8.68585	-8.685852	0.0000000
5	13	-8.68585	-8.685852	0.0000000
6	13	-8.68585	-8.685852	0.0000000
7	13	-8.68585	-8.685852	0.0000000
8	13	-8.68585	-8.685852	0.0000000
9	13	-8.68585	-8.685852	0.0000000
10	13	-8.68585	-8.685852	0.0000000
11	13	-8.68585	-8.685852	0.0000000

Table 5 : EKT Optimization for Gallium-arsenide LDA

EKT	Number of iterations	Total energy (E_T)	Harris energy (E_H)	ABS(E_T-E_H)
0.01	13	-8.6858517	-8.6858517	0.0000000
0.02	13	-8.6858517	-8.6858517	0.0000000
0.03	13	-8.6858516	-8.6858517	0.0000001

0.04	13	-8.6858517	-8.6858517	0.0000000
0.05	13	-8.6858517	-8.6858517	0.0000000
0.06	13	-8.6858516	-8.6858516	0.0000000
0.07	13	-8.6858513	-8.6858514	0.0000001
0.08	13	-8.6858505	-8.6858504	0.0000001
0.09	13	-8.6858485	-8.6858484	0.0000001
0.1	13	-8.6858446	-8.6858446	0.0000000

Table 6 : Summary of Optimal Values

Parameters	Gallium-arsenide
Delt	30
Gamma	0.2
Ecut	17
Ecuti	14
EKT	0.05
ldyn	2
i_dyn	2
t-metal	True
force eps	0.0001
ion_damp	tfor- false tsdp- false
ion_fac	No effect

b) Total energy calculations for GaAs using optimized parameters

Table 7 : Total energy calculation for bulk GaAs LDA

Number of iterations	Total Energy (E_T)
1	-8.6594317
2	-8.6608468
3	-8.6610073
4	-8.6610704
5	-8.6610831
6	-8.6610916
7	-8.6610937
8	-8.6610951
9	-8.6610935
10	-8.6610938
11	-8.6610948
12	-8.6610955
13	-8.6610957
14	-8.6610958

c) Graphs of Optimized Bulk Gallium-Arsenide using Fhi98md Input Variables

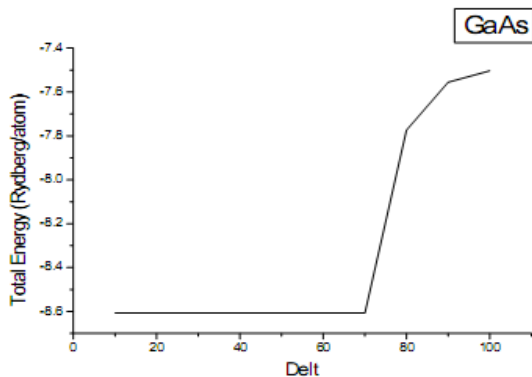


Figure 1 : Delt vs total energy (LDA) for GaAs

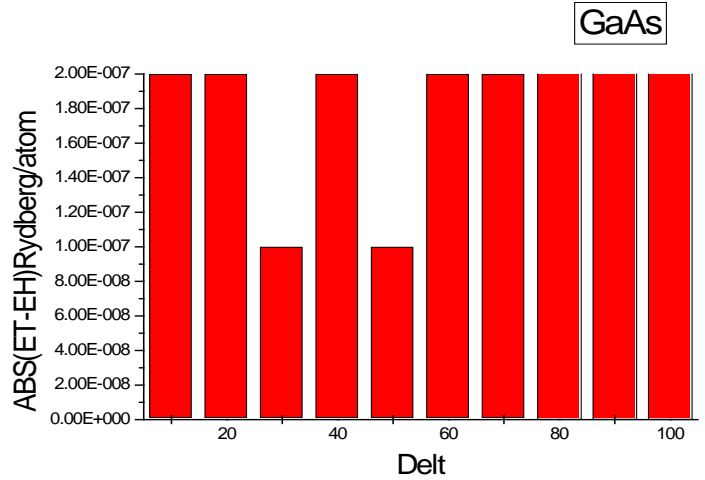


Figure 2 : Delt Vs Absolute difference between the Total energy and Harris Energy (LDA) for GaAs

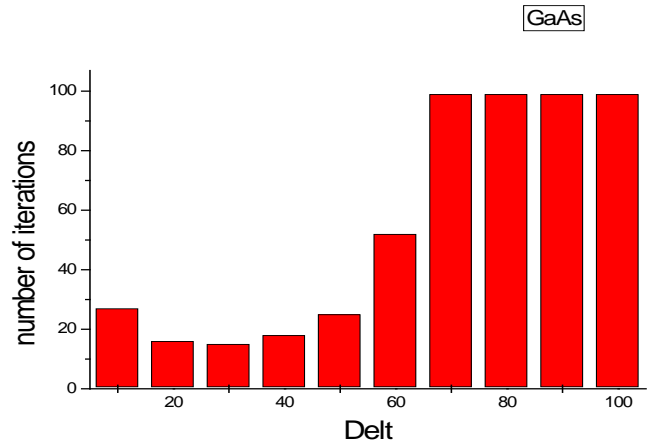


Figure 3 : Delt Vs number of iteration (LDA) for GaAs

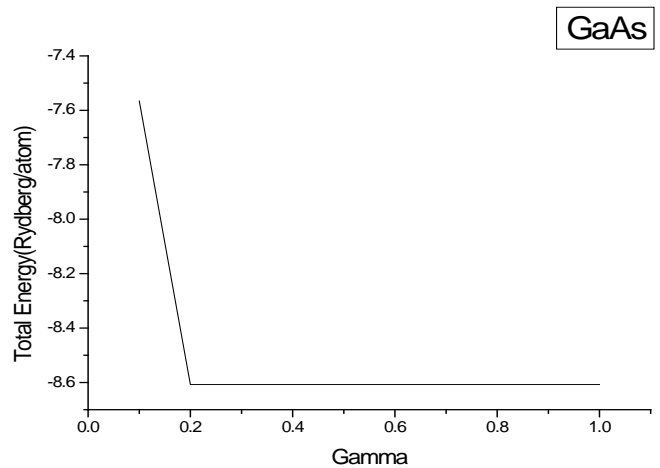


Figure 4 : Gamma vs. total energy (LDA) for GaAs

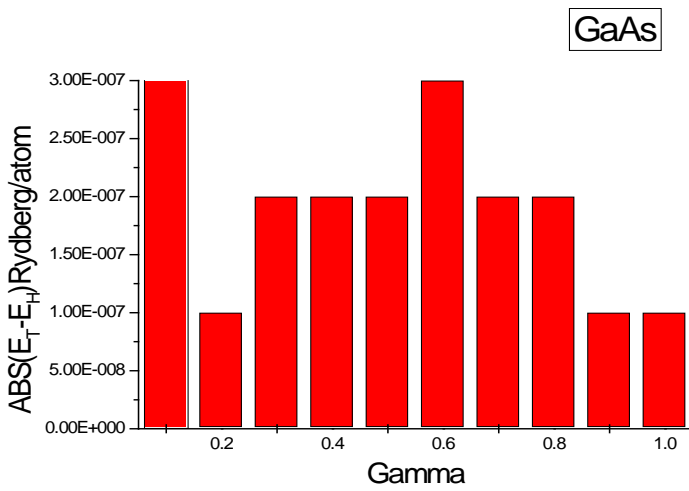


Figure 5 : Gamma Vs Absolute difference between the Total energy and Harris Energy (LDA) for GaAs

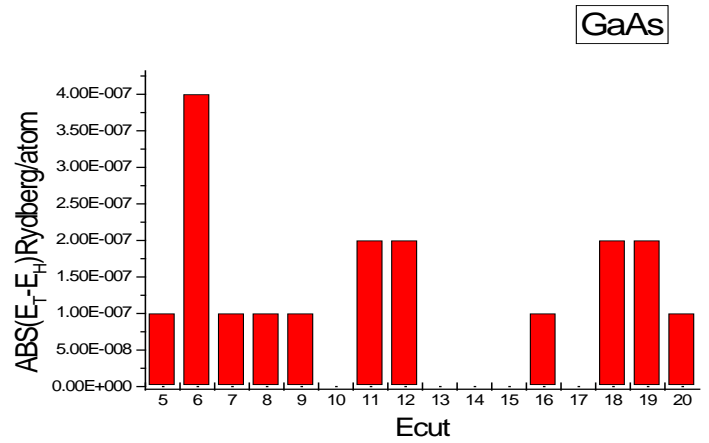


Figure 8 : Ecut Vs Absolute difference between the Total energy and Harris Energy (LDA) for GaAs

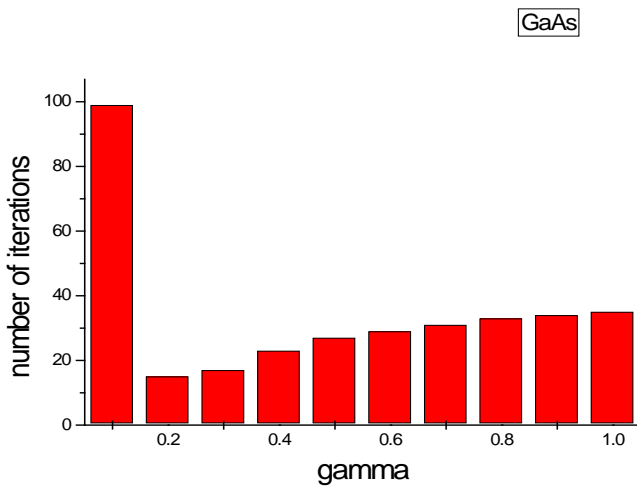


Figure 6 : Gamma Vs number of iterations (LDA) for GaAs

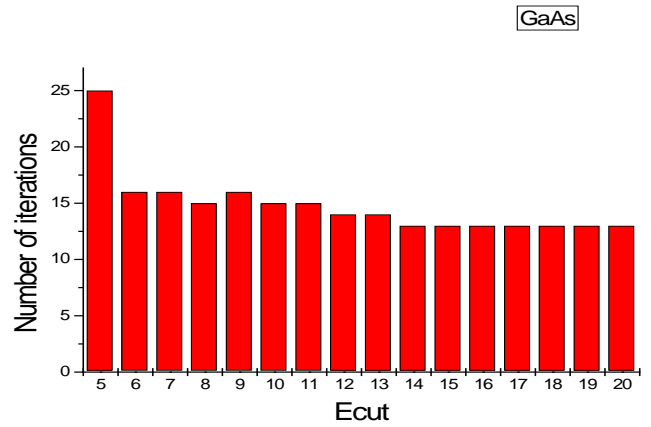


Figure 9 : Ecut Vs number of iterations (LDA) for GaAs

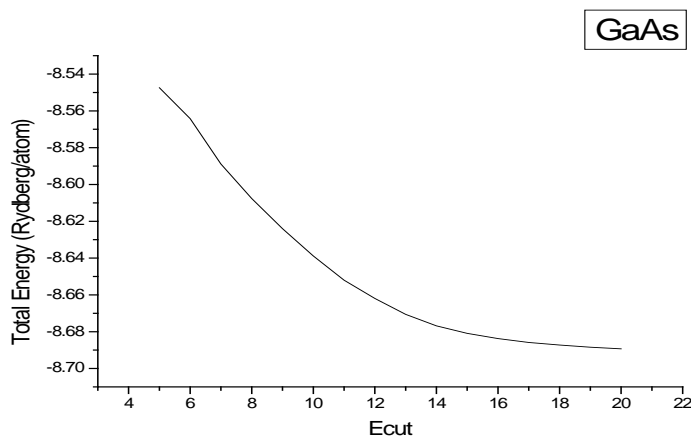


Figure 7 : Ecut Vs total energy (LDA) for GaAs

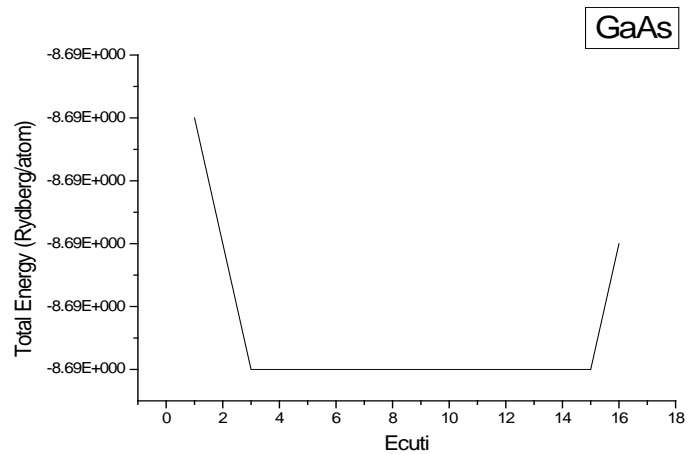


Figure 10 : Ecuti vs Total energy (LDA) for GaAs

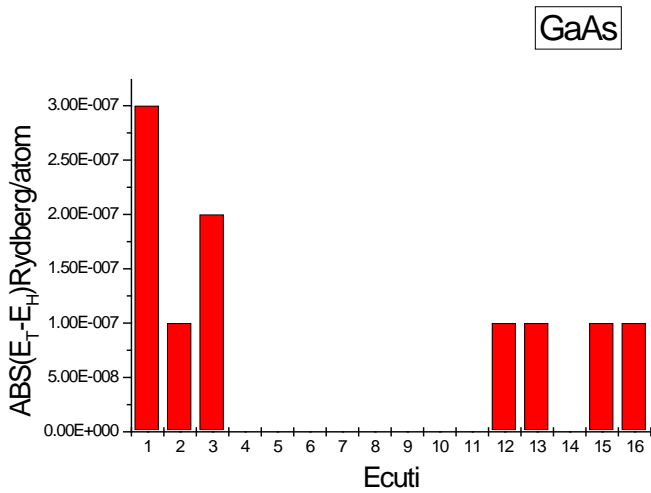


Figure 11 : Ecuti Vs Absolute difference between the Total energy and Harris Energy (LDA) for GaAs

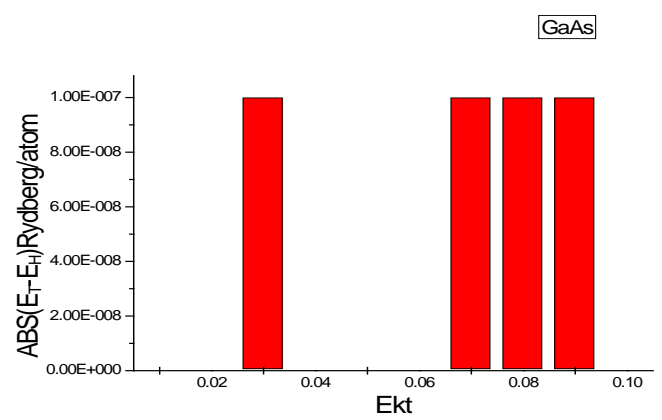


Figure 14 : Ekt Vs Absolute difference between the Total energy and Harris Energy (LDA) for GaAs

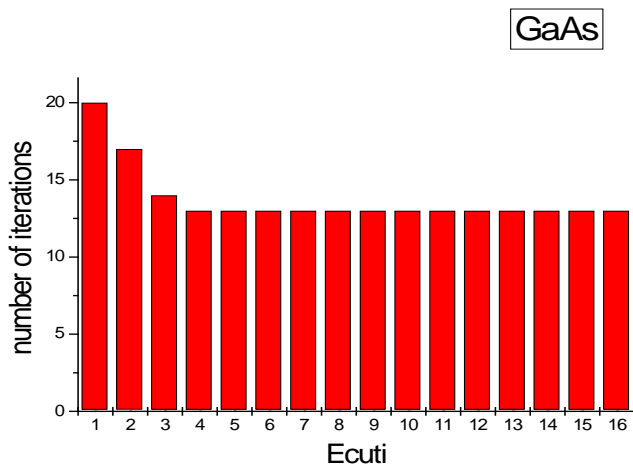


Figure 12 : Ecuti Vs number of iterations (LDA) for GaAs

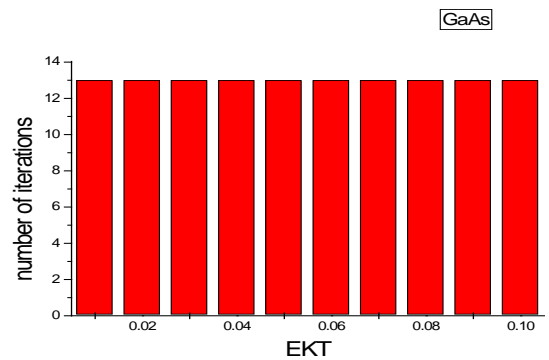


Figure 15 : Ekt Vs number of iterations (LDA) for GaAs

i. Total energy calculations for bulk GaAs

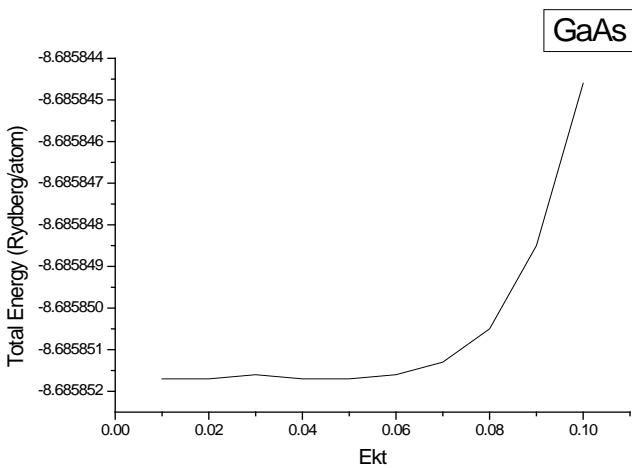


Figure 13 : Ekt vs Total energy (LDA) for GaAs

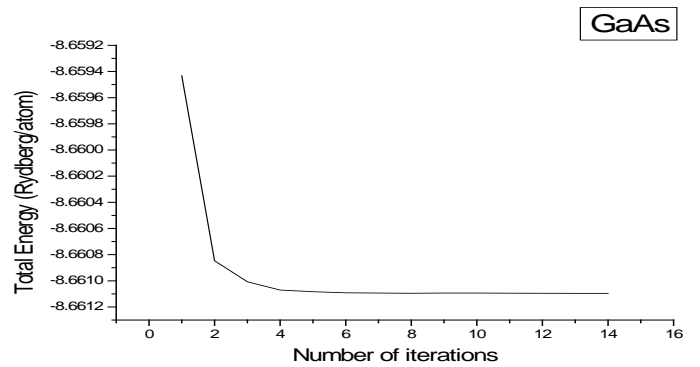


Figure 16 : Bulk Gallium-Arsenide convergence test (LDA)

IV. DISCUSSIONS

Fig1. Shows that Delt has a minimum energy between 10 and 70 while in Fig 2, Delt gave a more accurate result at 30 and 50. But from Fig 3 we can see that Delt has the least number of iterations at 30. This implies that 30 is the optimal value for Delt. However, fig 4 gave the minimum energy between 0.2 to 1.0 for Gamma, while fig 6 shows the least number of iterations

at 0.2 indicating that the optimal value for Gamma is 0.2. Fig 7-9 show that 17 is the optimal value for Ecut, while in figs 10-12 we can see that 14 is the optimal value for Ecuti. Fig: 16 show the bulk convergence test for GaAs which shows that the computations converged with total energy of -8.6610957 Rydberg/atom for GaAs.

This optimal values obtained for the parameters were used to calculate the total energy for bulk Gallium-arsenide. The energy -8.6610957 Rydberg/atom obtained for GaAs is in agreement with previously reported local density approximation (LDA) values of -8.0691176 Rydberg/atom (Stadele et al, 1999); and -8.364 Rydberg/atom. (Grzegoizewski, 2003).

V. CONCLUSION

The seven main parameters that determine electronic as well as structural convergence have been successfully optimized and the optimal values were used to calculate the bulk total energy of Gallium-arsenide: -8.6610757 Rydberg / atom for LDA. This is in agreement with previously reported theoretical values.

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