What is the most stable oxygen vacancy in β-Ga_2O_3?

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Abstract

Contents

1 Introduction

In my master thesis I will look at n-type dopant diffusion in the semiconductor β-Ga_2O_3. This diffusion is believed to be oxygen vacancy aided and dependent. In this project the three different oxygen vacancies in β-Ga_2O_3 was studied with density functional theory.

We started with convergence tests of the primitive unit β-Ga_2O_3, both with respect to cut-off energy and k-point density. We also looked at the density of states and plotted the band structure of β-Ga_2O_3.

After that, we increased the unit cell size to a super cell. This, to be able to insert an oxygen vacancy. We relaxed the structure and calculated the energy of the bulk β-Ga_2O_3.

After that we made three different supercells each with an oxygen vacancy at different oxygen sites. We relaxed the structure and then calculated the total energy. To find the formation energy of the different oxygen vacancies, the energy of an oxygen molecule in vacuum was calculated as well.

At last local density of state and electron density isosurfaces was used to investigate the oxygen vacancy further.

2 Theory

2.1 The material, β-Ga_2O_3

The primitive unit cell of β-Ga_2O_3 is base-centered monoclinic with the unit cell parameters listed in Table 2.1, which is in the space group C2/m. The structure has three inequivalent oxygen sites and two inequivalent gallium sites. The unit cell is shown in Figure 2.1. The oxygen sites are named O(I), (OII) and O(III). O(I) and O(II) are threefold coordinated, while O(III) is fourfold coordinated (see Figure 2.2). The gallium sites are called Ga(I) and Ga(II). Ga(I) and Ga(II) are tetrahedrally and octahedrally coordinated, respectively [1]. Figure 2.3 shows the different sites in the super cell. Figure 2.4 shows which gallium atoms the 'different' oxygens are bonded to and the length of the bonds. The lengths are from the relaxed super cell.

Table 2.1: This is the unit cell parameters for the β-Ga_2O_3 primitive unit cell.

a = 12.23000 Å	α = 90.0000°
b = 3.04000 Å	β =103.7000 °
c = 5.80000 Å	γ = 90.0000 °
V = 209.5042 $Å^3$	

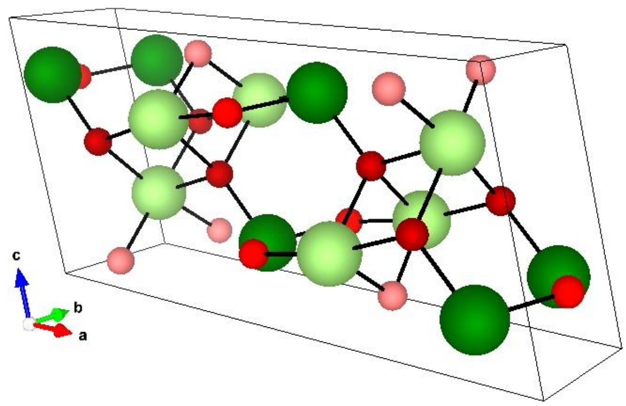


Figure 2.1: This figure shows the primitive unit cell of β-Ga_2O_3.

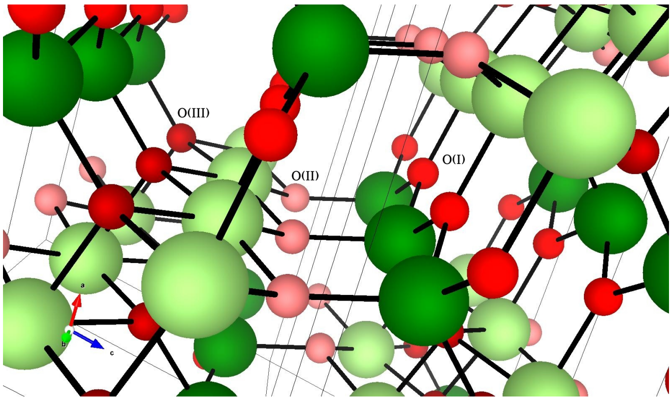


Figure 2.2: This figure shows the inequivalent oxygens in the unit cell. There are three different oxygen sites, they are color coded and named.

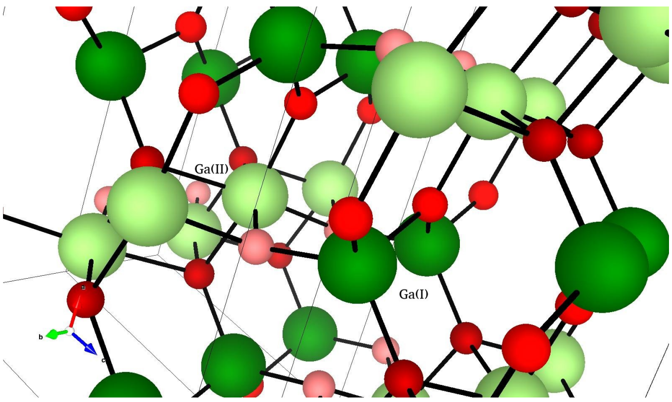


Figure 2.3: This figure shows the inequivalent gallium sites in the unit cell.

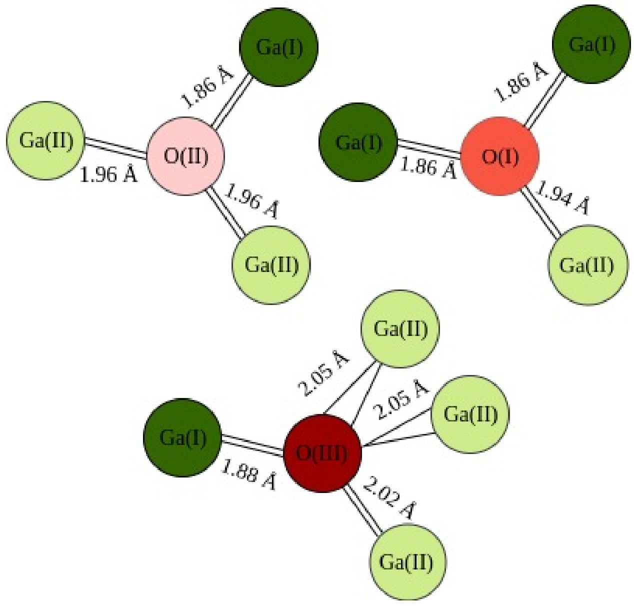


Figure 2.4: This figure shows the distances at the different oxygen sites in the relaxed super cell. We assume that the distances are similar for all equivalent sites in the super-cell, because these are the distances for a three specific ones.

2.2 DFT Convergence

The first thing one does when doing DFT calculations are convergence tests. This is important because it gives data one can use to consider how accurate the resulting properties will be, compared to how costly the calculations are. The more accurate results, the higher cost in CPU time. A convergence test will also show if numerical noise gives a limit to the accuracy of the result.

The convergence of a relative change in energy, relative change in force and relative change in pressure versus energy cut-off and k-point density is checked. The energy cut-off is a value that represent the limit of the infinite sum over G-vectors (see Equation 1). We cannot sum an infinite sum, so we have to choose a limit that is sufficient for the accuracy we want to achieve. Because it is a sum over G-vectors, the energy cut-off has to be big for localized states. Oxygen has localized states and that indicates that this material need a high energy cut-off for good accuracy.

$$E_{cut-off} = \sum \frac{1}{G} \qquad (1)$$

The k-point density is related to the k-point mesh of the numerical integral over k-vectors. Because it involves k-vectors it is related to more unlocalized states and metallic materials might need high k-point density because of their electrons delocalized states. β-Ga_2O_3 is a semiconductor though and might not need a high k-point density.

The properties are chosen to be the relative change because it is easier to converge and the total energy from DFT calculations are not that interesting physically because it is not a physical number. It is simply a numerical one. The relative change in energy is interesting though because then one can compare different situation. The comparison is physically interesting because it is independent of the real total value.

After choosing a convergence criteria, the accuracy one wants or settles at, the energy cut-off and the k-point density can be used to relax the structure. When relaxing the structure, the program minimizes the maximum force felt by the the atoms in the structure and, if one chooses to, minimizes the pressure. The energy cut-off and the k-point density is used for all the calculations; relaxation, the total energy and density of states calculations.

2.3 DFT Formation Energy

When comparing total energies from DFT calculations, it is important to compare the energy for the same amount of atoms. That means that if one compares the energy of a material with the energy of the material with a vacancy, as we will do in this project, one has to add the energy of the atom giving the vacancy in vacuum. In this case the vacancy is an oxygen vacancy and the energy of an oxygen molecule in vacuum also has to be calculated. This difference will give the formation energy of the oxygen vacancy.

The formation energy of the oxygen vacancy is actually also dependent on the temperature, pressure and the charge of the vacancy. The equation for calculating the formation energy is given in Equation 2 where E_{vac} is the total bulk energy with the vacancy, E_b is the total bulk energy without the vacancy, P is the pressure, μ_O is the chemical potential of oxygen given by Equation 3. $E_{tot}^{O_2}$ is the total energy of the oxygen molecule in vacuum, $\tilde{\mu}_{O_2}$ is the difference from $T = 0$ K at the reference pressure, P_0, and can be found in tables, $kT\log(\frac{P}{P_0})$ represents the difference in pressure, P, form the reference pressure and the last term represent the impact of a charged vacancy where q is the charge, ϵ_f is the Fermi level (or energy **??**) and ϵ_{VBM} is the maximum of the valence band.

$$E_f = (E_{vac} + \sum_i N_i \mu_i) - E_b + q(\epsilon_F + \epsilon_{VBM}) \quad (2)$$

$$\mu_O = \frac{1}{2}\mu_{O_2} = \frac{1}{2}\left(E_{tot}^{O_2} + \tilde{\mu}_{O_2} + kT\log(\frac{P}{P_0})\right) \quad (3)$$

In this project the setup is simple, the temperature is 0 K and the sample is assumed to be in oxygen rich conditions and in vacuum (how can it be in both o-rich and vacuum **??**). This makes the chemical potential of O_2, $\mu_{O_2} = E_{tot}^{O_2}$. The oxygen vacancy is also made to be neutral, not charged. A changed oxygen vacancy is a donor in the semiconductor, but if is is neutral the Fermi level is not changed and the term $q(\epsilon_F + \epsilon_{VBM}) = 0$. That is why the formation energy is simply given by Equation 4 where μ_O is simply given by Equation 5.

$$E_f = (E_{vac} + \mu_O) - E_b \quad (4)$$

$$\mu_O = \frac{1}{2}E_{tot}^{O_2} \quad (5)$$

3 Method

3.1 Set up

Type of GGA. VASP. PDE?

3.2 Execution

- Found structure for $\beta - Ga_2O_3$
- Checked convergence for energy cut off and k-point density for primitive unit cell
- Convergence criteria result:

  ENCUT = 600

  makekpoints -d 5 → (3x11x6)
- Relaxed the unit cell
- Plotted DOS and band structure for primitive unit cell
- Made super cell (1x 3y 2z)
- Changed convergence criteria:

  EDIFFG = -0.01

  ENCUT = 500

  ISIF = 3

  makekpoints -d 3 → (2x3x2)
- Relaxed super cell (both electronic and pressure)
- Calculated energy for relaxed unit cell
- Made three different structures for three different oxygen vacancies
- Relaxed all three structures
- Calculated energy for the relaxed structures
- Calculated energy of relaxed oxygen molecule in vacuum

  EDIFFG = -0.01

  EDIFF = 1E-5

  ENCUT = 500

  ISPIN = 2

  makekpoints -d 1 → (1x1x1)
- Found formation energy
- Plotted local DOS near vacancy and far away from it

3.3 Convergence

This section present the result from the convergence tests. The figures have normal convergence criteria plotted with the results, to help evaluate them.

3.3.1 Energy cut-off

$$|\Delta E_{rel}^i| = \left|\left(E_a^{i+1} - E_a^i\right) - \left(E_b^{i+1} - E_b^i\right)\right| \quad (6)$$

We started with convergence with respect to energy cut-off. Figure 3.1 shows the plot of the change in relative energy, ΔE_{rel} (see Equation 6), between the total energy of the primitive unit cell, E_a, and the total energy of the unit cell with one less oxygen, E_b, against the cut-off energy. The plot shows that a cut-off energy of 600 eV would give a good convergence well below 1 meV for the energy.

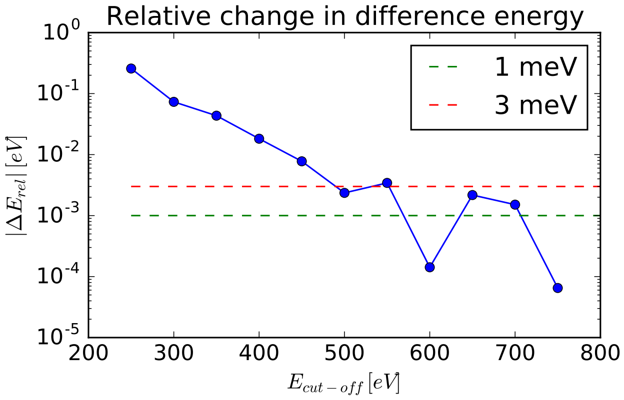


Figure 3.1: This is a plot of the difference between change in energy for β-Ga_2O_3 with and without a oxygen vacancy. We can see from the plot that a cut-off energy of 600 eV is sufficient.

We also looked at the force and the pressure with respect to the cut-off energy. Figure 3.2 shows the result. A cut-off energy of 600 eV gives a good convergence for force and pressure also.

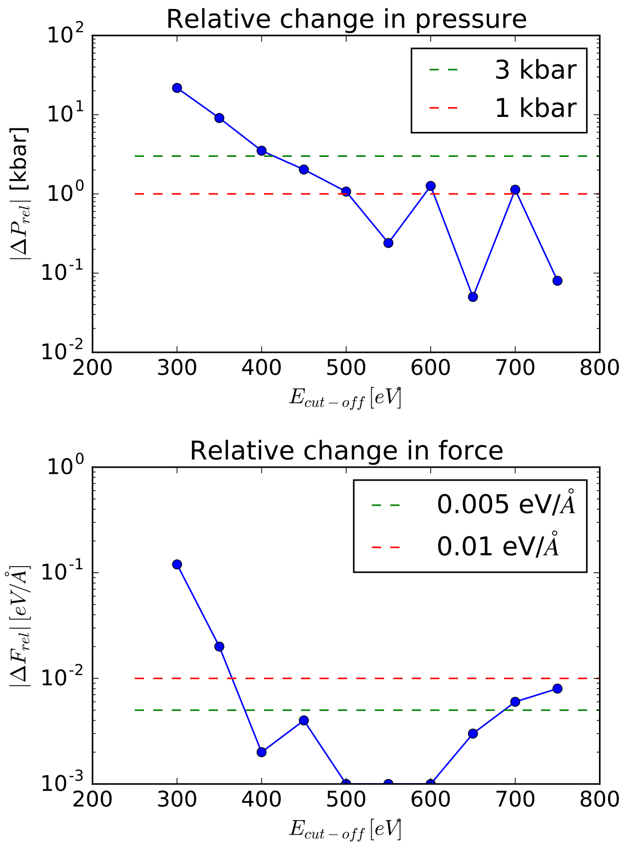


Figure 3.2: This is a plot of the difference between change in both force and pressure for β-Ga_2O_3 with and without a oxygen vacancy. We can see from the plot that with respect to pressure and force 600 eV is more than sufficient. The change in force increases, but it is still small.

After increasing the primitive unit cell to a super cell, the CPU time of the relaxation increased a lot. To make the calculations more workable, the convergence criteria was made a little less strict and the new cut-off energy was sat to 500 eV. When we look at Figure 3.1 and 3.2 we see that a cut-off energy at 500 eV gives a good convergence as well, it is still around 3 meV for the energy and around 1 kbar for the pressure and 0.01 eV/Å for the force.

3.3.2 k-point density

Thereafter, we evaluated the necessary k-point density. Figure 3.3 shows the result for the relative change in energy and Figure 3.4 tshows the same for force and pressure.

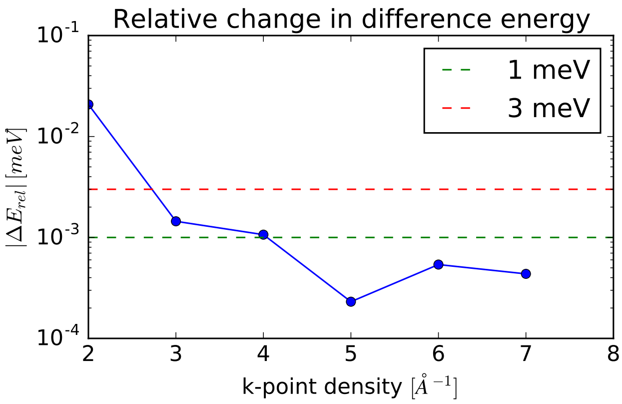


Figure 3.3: This is a plot of the difference between change in energy for Ga_2O_3 with and without a oxygen vacancy. We can see from the plot that a k-point density of 5 Å^{-1} is sufficient.

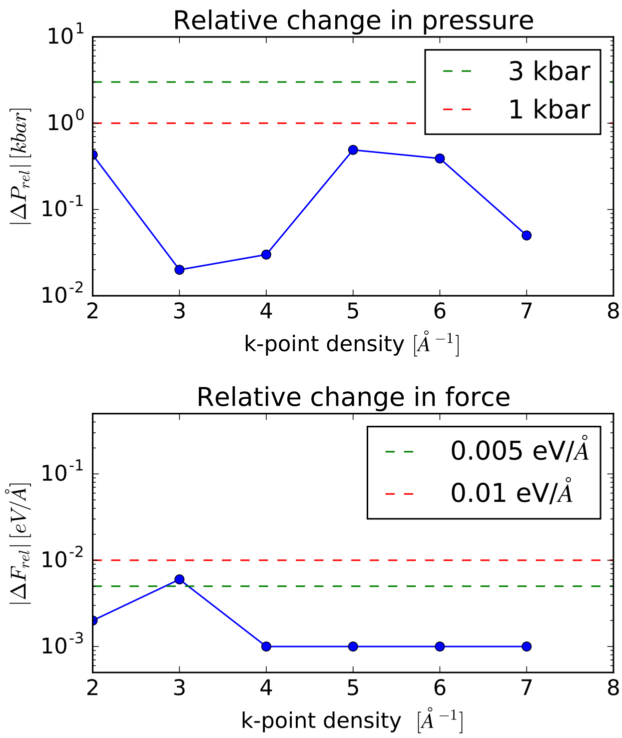


Figure 3.4: This is a plot of the difference between change in both force and pressure for Ga_2O_3 with and without a oxygen vacancy. All the k-point densities gives good convergence.

Initially the k-point density was put to 5 Å^{-1}, for the accuracy to be at 1 meV for the energy. After the change in strictness, only 3 Å^{-1} were necessary to accomplish the criteria of 3 meV for the accuracy of the energy, 1 kbar in pressure and 0.01 eV/Å in force.

4 Result and Discussion

The units and uncertainties of the properties in this section are set here. The energy unit is eV with uncertainty $\pm$ 0.003 eV, pressure is in units kbar with uncertainty $\pm$ 1 kbar and force in units eV/Å with uncertainty $\pm$ 0.01 eV/Å.

4.1 Primitive unit cell

With the initial decided convergence criteria and the resulting energy cut-off (600 eV) and k-point density (5 Å^{-1}), we relaxed the primitive unit cell. Table 4.1 shows both the maximum force and the pressure decreasing (ISIF = 3). The relaxation criteria for the force was set to -0.01 eV/Å (EDIFFG = -0.01).

Table 4.1: This table lists the start and stop of the relaxation of the primitive unit cell. Both the maximum force, F_{max}, and the pressure, P, is decreasing in the relaxation.

F_{max}	$\#atom$	P	Drift	E_{tot}
1.716	9	139.52	0.000	-119.461
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
0.006	9	0.42	0.000	-120.224

The total energy per atom with a primitive unit cell was $\frac{E_{tot}}{\#\text{ of atoms}} = \frac{-120.249\text{ eV}}{20} \simeq -6.013$ eV after the relaxation.

4.1.1 Density of States

To examine the different oxygen sites, the local density of states (DOS) was plotted for the inequivalent sites. The local DOS plots for the O(I), O(II) and O(III) are in Figure 4.4, Figure 4.2 and Figure 4.3 respectively.

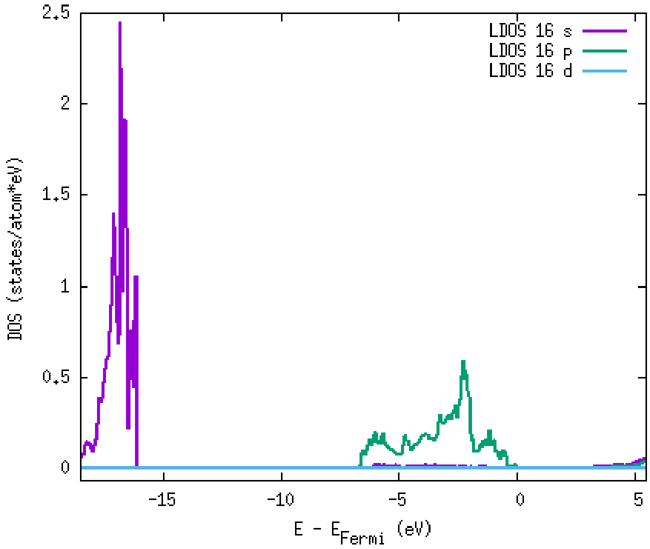


Figure 4.1: This is a plot of local density of states at the O(I) site.

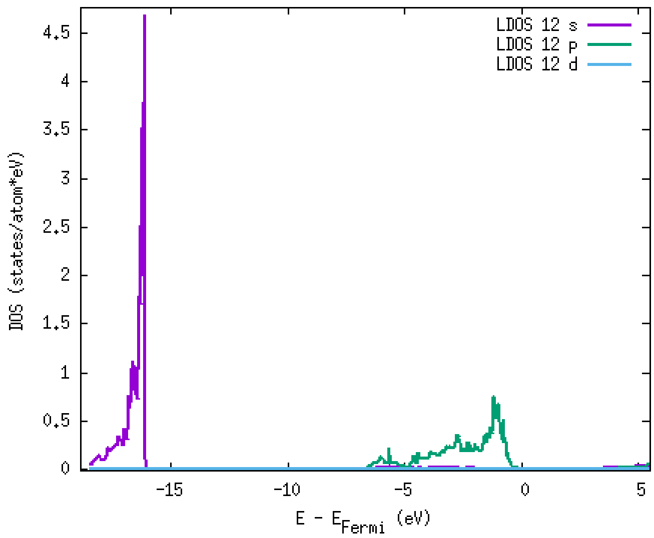


Figure 4.2: This is a plot of local density of states at the O(II) site.

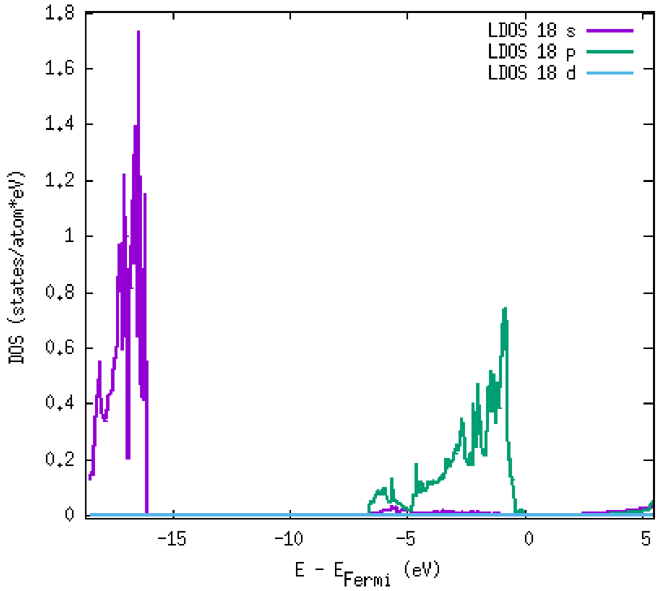


Figure 4.3: This is a plot of local density of states at the O(III) site.

The structure has two different gallium sites as well, and their local density of states are shown in Figure 4.4 and 4.5.

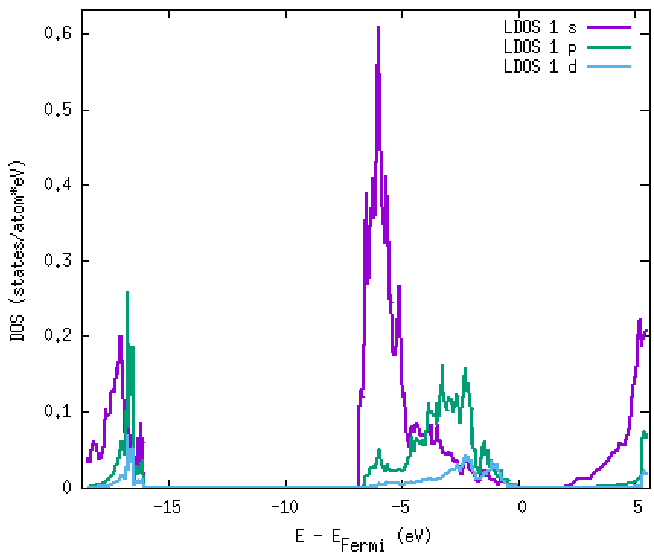


Figure 4.4: This is a plot of local density of state at the Ga(I) site.

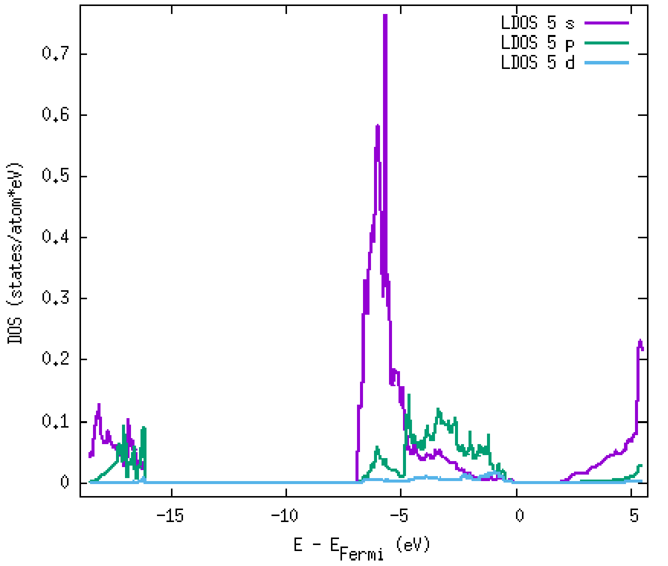


Figure 4.5: This is a plot of local density of state at the Ga(II) site.

In the theory we can see that all the oxygen sites are 'bonded' to both gallium sites, but the number of each bonds differ (see 2.4). The p-orbitals with energy, $E - E_{Fermi}$, from -15 eV to 0 eV are in all the local density plots, both the gallium ones and the oxygen ones, indicating bonds between them all. There are also s-orbitals below -17 eV in all plots. There are many states there at the oxygen sites and fewer at the gallium sites. The gallium local DOS plots show some states in the d-orbitals, but oxygen do not, and that is of course what we expect.

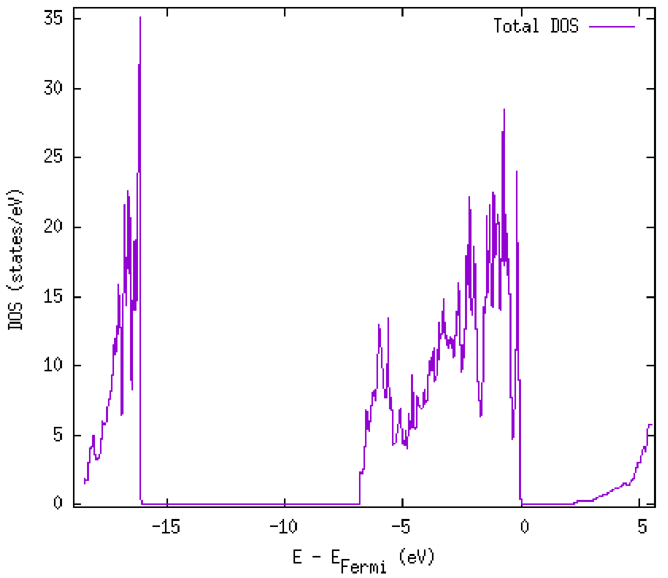


Figure 4.6: This is a plot of density of state of the primitive unit cell.

The total density of state of the primitive unit cell is plotted in Figure 4.6. The figures shows three bands in this energy interval, to bands below the Fermi level and the conduction band, of unoccupied states, as a semiconductor should have at temperature O K. The band gap is visual from 0 eV to around 2 eV, this is very small compared to experiments that gives the band gap at around 4.9 eV [1]. This is expected though because of the use of the simple GGA functional and no other compensation for the normal underestimation of band gap size.

4.1.2 Band structure

At last we plotted the band structure of β-Ga_2O_3. The band gap was found to be 1.8051 eV which is way too small. Figure 4.7 shows the band structure we plotted after our calculations. Figure 4.8 shows the band structure from an article where they used hybrid functionals and other tricks to get the correct band gap [1].

The band structure in Figure 4.7 shows that the lowest point in the conduction band is at the Γ-point (G), and this corresponds with the result in Figure 4.8. The highest point in the valence band on our band structure is difficult to set, but in the other it is either at the M-point or the Γ-point.

There seems to be something wrong at the M-point in our calculations because it looks very different form the other one. The band gap of β-Ga_2O_3 is indirect, but the difference in the valence band between the Γ-point and the M-point is so small, that it is practically direct [1].

Figure 4.7: This is a plot of the band structure of β-Ga_2O_3 form our density of states calculations.

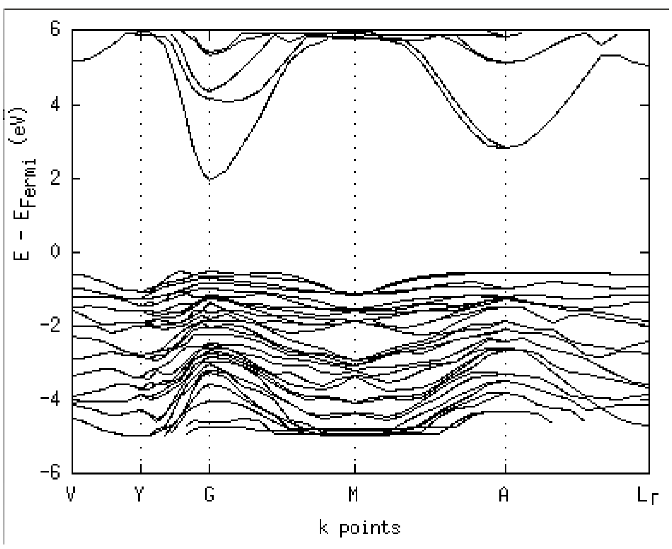
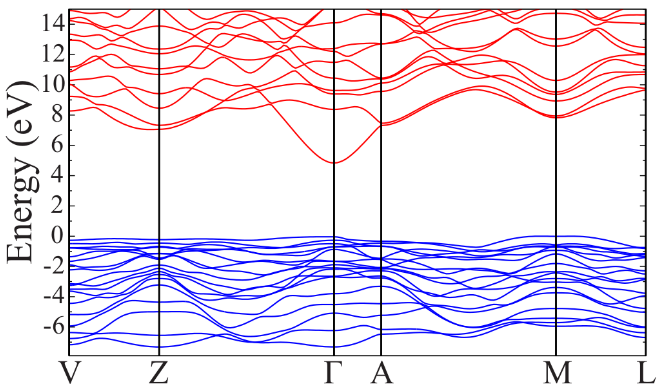


Figure 4.8: This is a plot of the band structure taken from an article that did DFT on β-Ga_2O_3 with hybrid density functionals [1].



4.2 Super cell

To be able to look at oxygen vacancies without getting extremely high concentrations of them, we increased the primitive cell to a super cell by adding two primitive cells in the y-direction (b-direction) and one in the z-direction (c-direction).

4.2.1 Relaxation and energy

Our first relaxation of the unit cell was done with the initial convergence results of an energy cut-off at 600 eV and a k-point density at 5 Å^{-1} giving a k-mesh of (3x4x3). The convergence for the maximum force was put to only -0.05 eV/Å (EDIFFG = -0.05) and we only relaxed the ions not the cell (ISIF = 2). The result of the relaxation is in Table 4.2.

Table 4.2: This table has the first and last relaxation step of supercell with the initial convergence result.

F_{max}	$\#atom$	P	Drift	E_{tot}
0.443	49	134.07	0.023	-718.260
⋮	⋮	⋮	⋮	⋮
0.009	25	109.22	0.023	-718.913
CPU	time:	3546.421 s		≈ 59 min

Because the pressure was so big, we wanted to relax the cell as well. We also wanted to decrease the convergence of the maximum force to 0.01 eV/Å (EDIFFG = -0.01) to match the convergence criteria of the force. Because the relaxation calculation was costly already, a decision to make the convergence criteria less strict was made. It was done like described earlier in the method part of this report. The total energy of the super cell after the initial relaxation is given in Table 4.3.

Energy calculation after:

Table 4.3: The energy output after relaxation of supercell with first relaxation result.

F_{max}	P	Drift	E_{tot}

4.2.2 Changed convergence criteria

The relaxation was then done with the changed convergence results with an energy cut-off at 500 eV and a k-point density at 3 Å^{-1} giving a k-mesh of (2x3x2). The convergence for the maximum force was put to -0.01 eV/Å (EDIFFG = -0.01) and we relaxed both the ions and the cell (ISIF = 3). The result of the relaxation is in Table 4.4 and the total energy of the super cell calculated from the relaxed structure is in Table 4.5.

Table 4.4: This table has the first and last relaxation step of supercell with the changed convergence criteria.

F_{max}	$\#atom$	P	Drift	E_{tot}
0.427	49	136.09	0.023	-717.821
⋮	⋮	⋮	⋮	⋮
0.006	49	0.03	0.024	-720.914

Table 4.5: The energy output after last relaxation of supercell.

F_{max}	P	Drift	E_{tot}
0.045	0.023	2.63	-721.081

The total energy per atom with the super cell was $\frac{E_{tot}}{\#\text{ of atoms}} = \frac{-721.081 \text{ eV}}{120} \simeq -6.009$ eV after the relaxation. The energy per atom is the same as for the primitive unit cell, within the chosen accuracy.

4.3 O_2 in vacuum

To calculate the formation energy we need the energy of oxygen in vacuum. This energy was calculated with the same cut-off energy as before and the k-point density 1 Å^{-1} which gives the k-mesh (1x1x1) because it is only one molecule with vacuum in all directions. O_2 has a paramagnetic ground state, so we had to turn on the spin -polarization (ISPIN = 2). We relaxed the structure (Table 4.6 and then calculated the total energy (see Table 4.7).

Table 4.6: This table has relaxation steps of $=_2$ in vacuum.

F_{max}	$\#_{atom}$	P	Drift	E_{tot}
0.087	1	-0.22	0.000	-9.883
0.406	1	0.09	0.000	-9.882
0.000	1	-0.16	0.000	-9.883

Table 4.7: The energy output of oxygen in vacuum.

F_{max}	P	Drift	E_{tot}

From this energy we can calculate the chemical potential, at our conditions, using Equation 5:

$$\mu_O = \frac{1}{2} E_{tot}^{O_2} = \frac{1}{2} \cdot (-9.883) = -4.942$$

4.4 The different oxygen vacancies

Furthermore, we removed an oxygen atom from the three different sites, relaxed the structures and calculated the total energy of the structures. The same parameters were used in these as the calculations of the super cell without vacancies.

4.4.1 Relaxation

Table 4.8 shows the first and last ionstep of the relaxation of the super cell with a O(I) vacancy. Table 4.9 and Table 4.10 shows the same for the O(II) vacancy and the O(III) vacancy respectively.

Table 4.8: The ionstep - relaxation of super cell with O(I) vacancy.

F_{max}	$\#_{atom}$	P	Drift	E_{tot}
2.666	19	133.08	0.142	-708.492
⋮	⋮	⋮	⋮	⋮
0.032	63	-0.03	0.465	-712.142

Table 4.9: The ionstep - relaxation of super cell with O(II) vacancy.

F_{max}	$\#_{atom}$	P	Drift	E_{tot}
2.391	20	135.21	0.010	-708.256
⋮	⋮	⋮	⋮	⋮
0.013	60	-0.01	0.143	-711.709

Table 4.10: The ionstep - relaxation of super cell with O(III) vacancy.

F_{max}	$\#_{atom}$	P	Drift	E_{tot}
1.873	1	135.42	0.141	-707.966
⋮	⋮	⋮	⋮	⋮
0.017	73	-0.00	0.145	-711.463

4.4.2 Total Energy

The total energy and other output of the relaxed structures are in Table 4.11.

Table 4.11: The energy output after relaxation of supercell with oxygen vacancies.

Vacancy	F_{max}	P	Drift	E_{tot}
O(I)	0.107	0.146	2.29	-712.283
O(II)	0.067	0.198	2.39	-711.860
O(III)	0.087	0.221	2.13	-711.603

4.4.3 Formation Energy

We used Equation 4 to calculate the formation energy of the three different situations and find which of the vacancies that had the smallest formation energy.

Table 4.12: This is the calculated formation energies for the diffrent oxygen vacancies at oxygen rich conditions. E_f is the formation energy, E_{vac} is the total bulk energy with the spesicied vacancy, E_b is the total bulk energy without a vacancy and μ_O is the chemical potential of oxygen.

Vacancy	$(E_{vac} + \mu_O) - E_b =$	E_f
O(I)	$(-712.282 - 4.942) - 721.081 =$	3.857
O(II)	$(-711.860 - 4.942) - 721.081 =$	4.279
O(III)	$(-711.603 - 4.942) - 721.081 =$	4.536

From Table 4.12 we can read that the O(I) vacancy has the lowest formation energy at the conditions we are checking at.

4.5 Why the O(I) vacancy?

We will use isosurfaces and local DOS to evaluate why the O(I) vacancy is the one with smallest formation energy.

4.5.1 Total density of states

First we can see that a defect level has showed up in the band gap, probably from the oxygen vacancy. This is shown when comparing Figure 4.9 which is the total DOS of the supercell without vacancies and 4.10 which is DOS of the supercell with the O(I) vacancy.

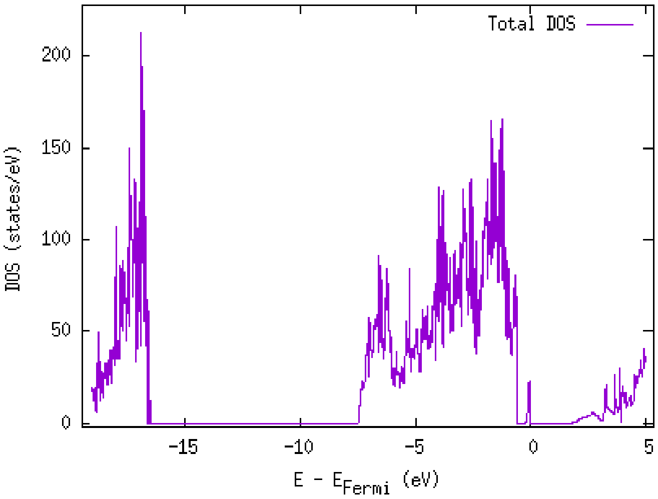


Figure 4.9: This is a plot of the density of state of the super cell with a O(I) vacancy.

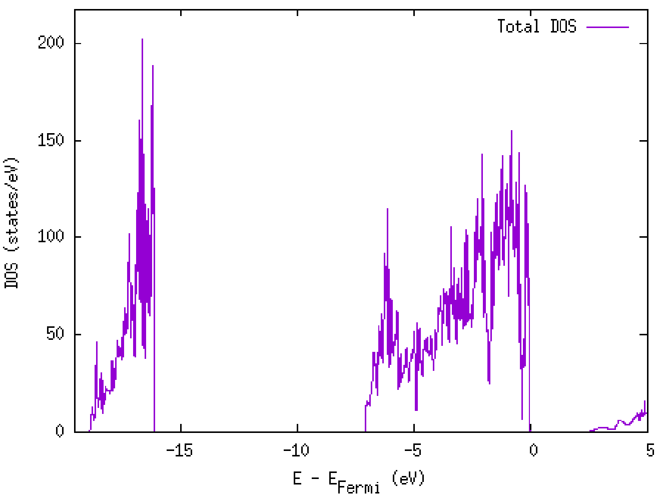


Figure 4.10: This is a plot of density of state of the general supercell.

4.5.2 Isosurfaces

Figure 4.11 shows the structure around the O(I) vacancy with different electron density isosurface levels. When the isosurface level is set to 0.04, an electron density is visible between the two Ga(I) atoms the O(I) atom should have been bonded to and and when the isosurface level is 0.03, the isosurface shows a bond between them (Figure 4.12).

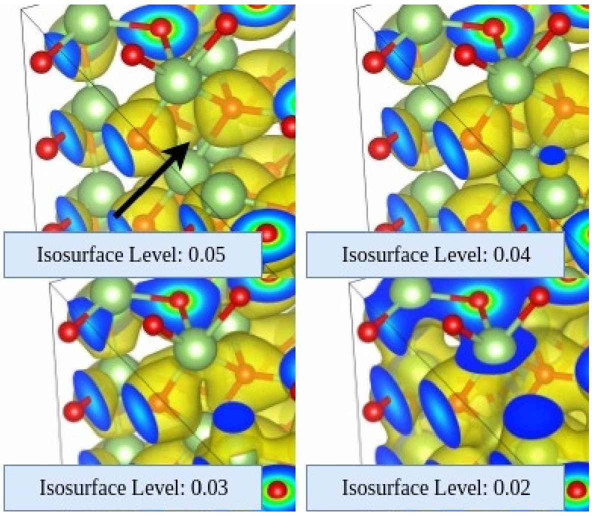


Figure 4.11: This figure shows the O(I) vacancy with different electron density isosurfaces.The black arrow points to the O(I) vacancy. When the isosurface level is lowered, a bond appears between the two Ga(I) atoms the O(I) should have been bonded to (Figure 4.12).

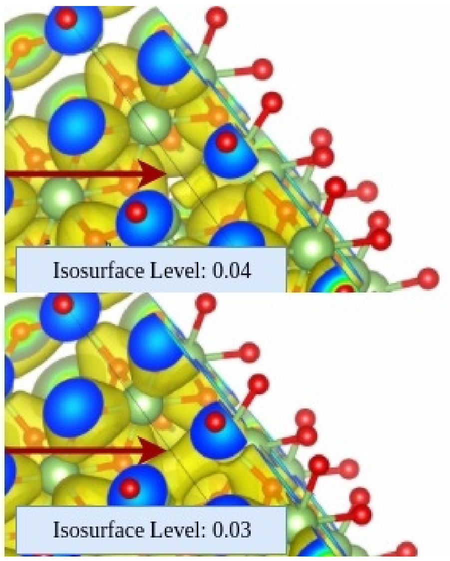


Figure 4.12: This figure shows the oxygen vacancy with different isosurfaces.In this figure the bond between the two Ga(I) atoms shows clearly. The isosurface goes from one atom to the other at the isosurface level 0.03.

Figure 4.13 shows the O(II) vacancy with different isosurfaces, when the isosurface level is lowered, the electron density around the Ga(I)-atom shows. The 'blob' shows the dangling bonds at the Ga(I) atom, but there is no 'blob' at the Ga(II) atoms. With the O(II) vacancy the isosurface level needs to be 0.02 for there to be a connection with the other Ga(II) atoms.

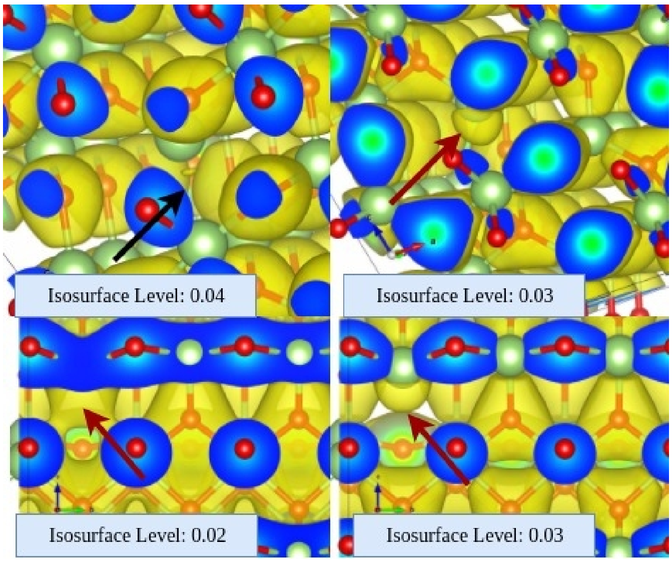


Figure 4.13: This figure shows the O(II) vacancy with different electron density isosurfaces.The figure shows the oxygen vacancy from different angles. The black arrow points to the vacancy and the red arrows points to the isosurface indicating dangling bonds at the Ga(I) atom.

Figure 4.14 shows the same for the O(III) vacancy. As in the case for the O(II) vacancy, the isosurface level needs to be 0.02 before there is a connection, and before that there is the same 'blob' at the one Ga(I) atom, indication dangling bonds.

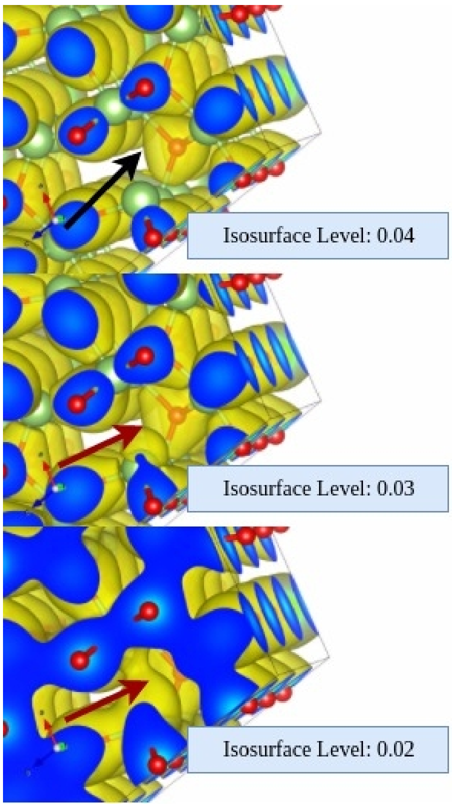


Figure 4.14: This figure shows the oxygen vacancy with different electron density isosurfaces.The black arrow points to the oxygen vacancy and the red arrows points to the dangling bond at the Ga(I) atom.

The difference between the O(I) vacancy with two Ga(I) atoms, that seems to form a covalent bond in the absence of an oxygen, and the other two vacancies, that only have one Ga(I) atom, might be a reason why the O(I) vacancy has the lowest formation energy.

The reason for the bond between two the Ga(I) atoms may come from the shorter length of the O-Ga(I) bond compared to the O-Ga(II) bond (see Figure 2.4). The 'bulb' from the isosurface always occur at the Ga(I) atom, and nothing at the Ga(II) atoms. Maybe the Ga(I) atom has dangling bonds, and the Ga(II) relocate the electrons elsewhere, making the O(I) more stable because the dangling bonds are in a bond instead.

4.5.3 Local DOS Ga(II)

lDOS - bredden sier om båndene er bånd - ikke så lokaliserte. Bånd til venstre er mer stabile - lenger borte fra fermi nivået.

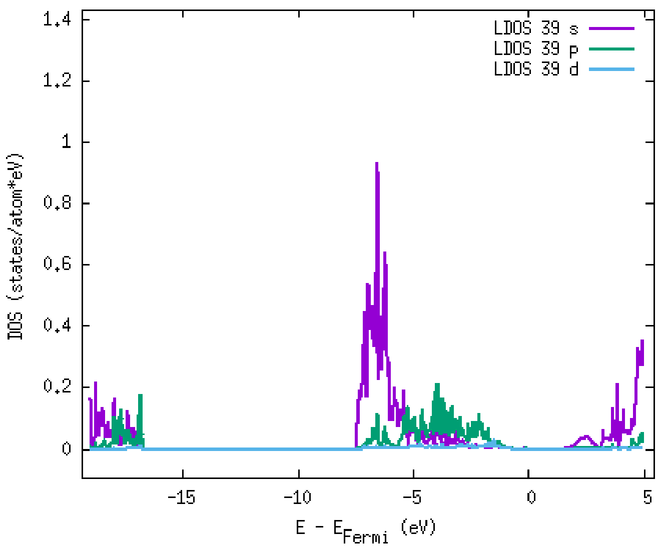


Figure 4.15: This is a plot of local density of state at the Ga(II) site next to the O(I) vacancy in the super cell.

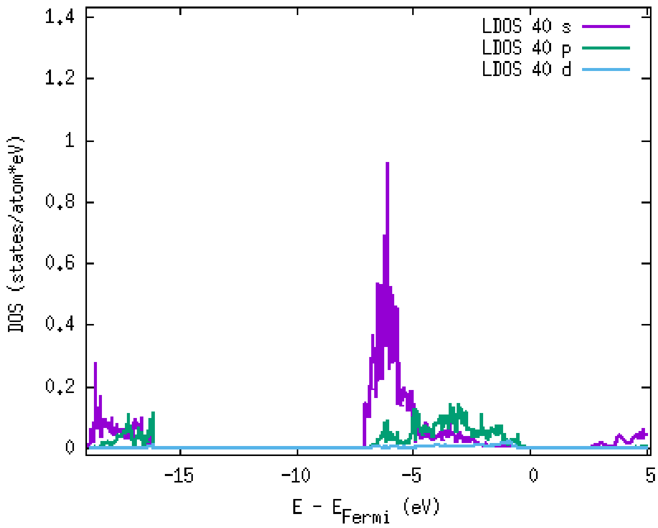


Figure 4.16: This is a plot of local density of state at the Ga(II) site in the general supercell.

4.5.4 Local DOS Ga(I)$_1$

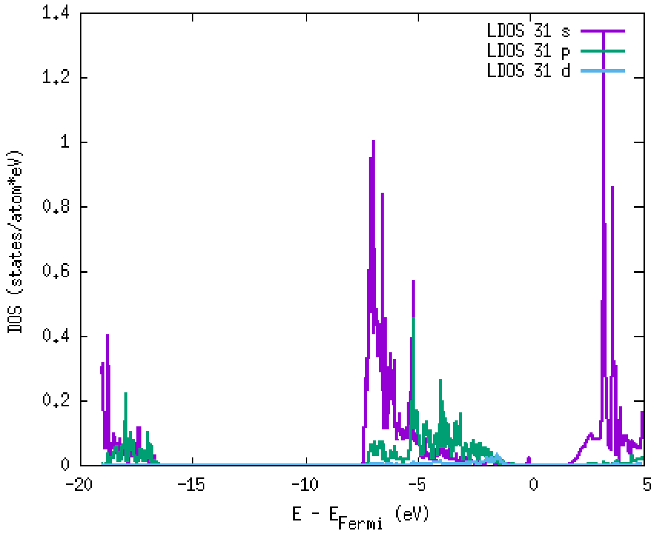


Figure 4.17: This is a plot of local density of state at the Ga(I) site next to the O(I) vacancy in the super cell.

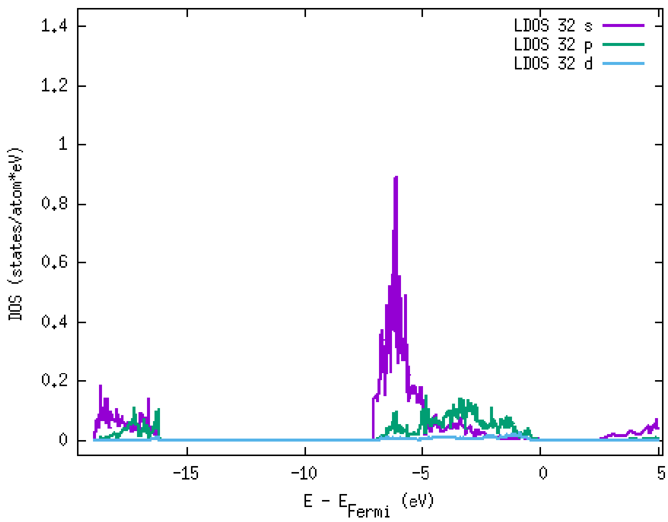


Figure 4.18: This is a plot of local density of state at the Ga(I) site in the general supercell.

4.5.5 Bond between Ga(I)$_1$ and Ga(I)$_2$?

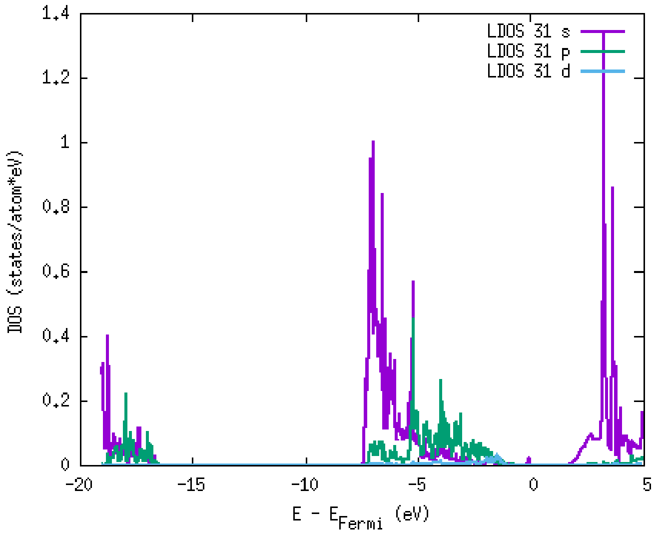


Figure 4.19: This is a plot of local density of state at the Ga(I) site next to the O(I) vacancy in the super cell.

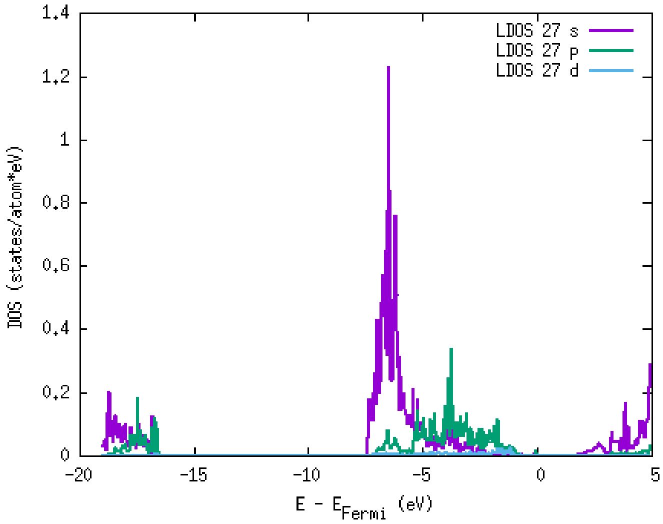


Figure 4.20: This is a plot of local density of state at the other Ga(I) site next to the O(I) vacancy in the super cell.

5 Conclusion

References

[1] JB Varley, JR Weber, A Janotti, and CG Van de Walle. Oxygen vacancies and donor impurities in β-Ga_2O_3. *Applied Physics Letters*, 97(14):142106, 2010.

Appendix