Project FYS-MENA 4111 β-Ga_2O_3

Vilde Mari Reinertsen

November 8, 2017

Abstract

Contents

1 Introduction **2**
1.1 Motive . . . 2
1.2 To do . . . 2

2 Theory **3**

3 Method **3**
3.1 Energy convergence . . . 3
3.1.1 Energy cut-off . . . 3
3.1.2 k-point density . . . 3
3.1.3 CPU time . . . 3

4 Result **3**

5 Discussion **3**

6 Conclusion **3**

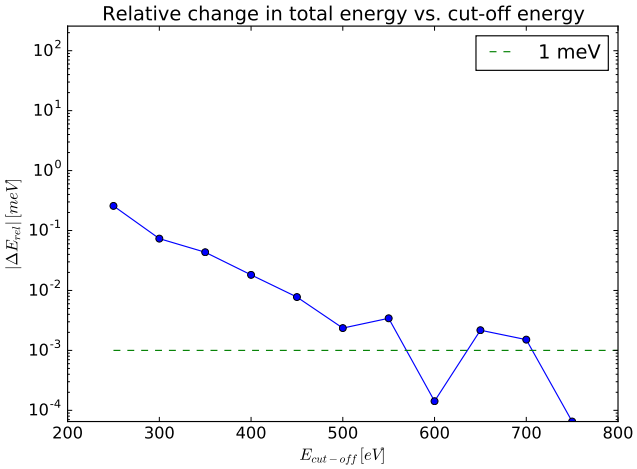

Figure 3.1: This is a plot of the difference between change in energy for Ga_2O_3 with and without a oxygen vacancy. We can see from the plot that a cut-off energy of 600 eV is sufficient. Include the criteria?

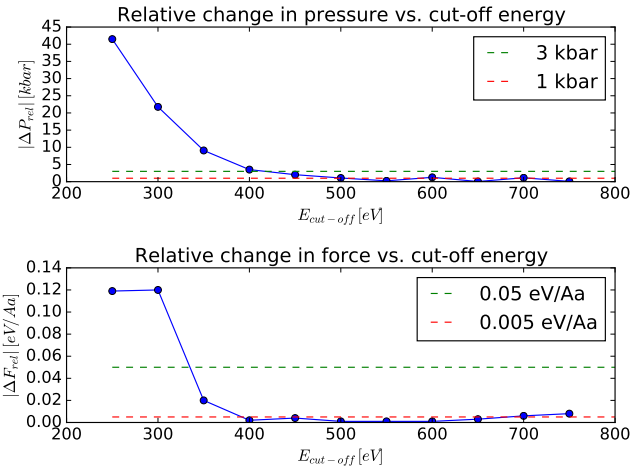

Figure 3.2: This is a plot of the difference between change in both force and pressure for Ga_2O_3 with and without a oxygen vacancy. We can see from the plot that with respect to pressure and force 600 eV is more than sufficient.

1 Introduction

1.1 Motive

1.2 To do

Use primitive unit cell base-centered monoclinic.

Start by checking convergence of the energy cut-off (400 eV).

(Remember to check relative also)

Convergence of k-points - 2, 3, 4, 5, 6, 7 (4 is often good)

Look at band structure.

Look at Si-donor, Sn-donor, H-donor, O-vacancy?

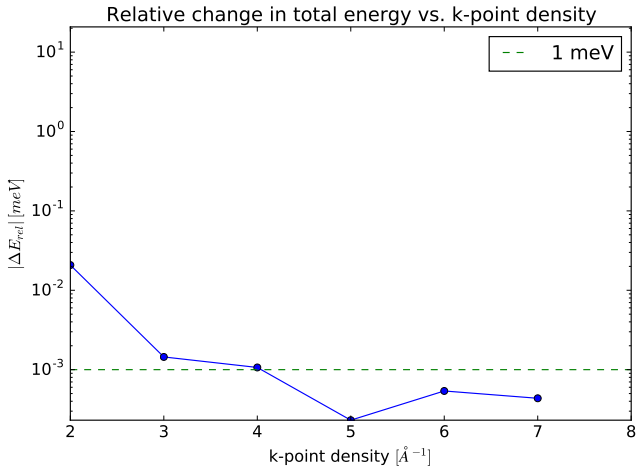

Figure 3.3: This is a plot of the difference between change in energy for Ga_2O_3 with and without a oxygen vacancy. We can see from the plot that a k-point density of 5 $Å^{-1}$ is sufficient.

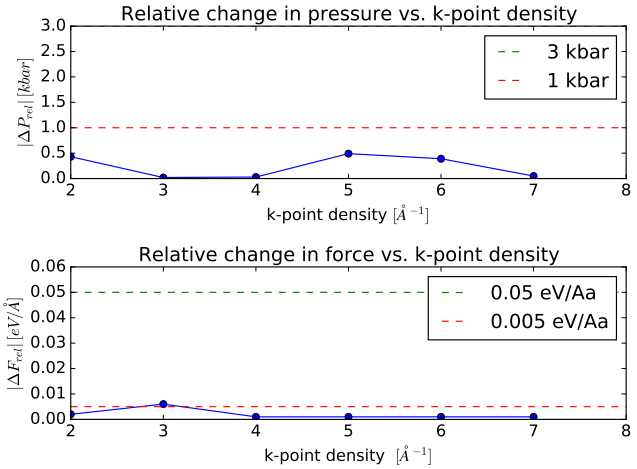

Figure 3.4: This is a plot of the difference between change in both force and pressure for Ga_2O_3 with and without a oxygen vacancy. Are the same criterias ok?

Table 3.1: Caption

k-point density [Å^1]	Total CPU time [s]
2	6.479
3	11.657
4	18.80
5	27.572
6	50.383
7	65.509
8	94.243

2 Theory

3 Method

3.1 Energy convergence

3.1.1 Energy cut-off

3.1.2 k-point density

3.1.3 CPU time

Forandret avstandene seg etter relax?

Band gap:

Gap Band# VBM CBM VBM-occ CBM-occ 2.3532 48 1.9458 4.299 2.0 0.0

4 Result

5 Discussion

6 Conclusion

Appendix

VESTA: K. Momma and F. Izumi, "VESTA 3 for three-dimensional visualization of crystal, volumetric and morphology data," J. Appl. Crystallogr., 44, 1272-1276 (2011).