Density Functional Theory Analysis of AlMgB14

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Introduction

Aluminum Magnesium Boride is a newer material with a lot of fascinating properties. AlMgB14 has a lower friction coefficient than ice, it is among the hardest materials known and is very resistive to wear. There is great interest in the material for various uses such as potential heat shielding applications for NASA and neutron shielding in nuclear reactors.

AlMgB14 has not been thoroughly studied, and its material and atomic properties have not been determined. There have been several conflicting results from a small number of studies. The main conflicting result is whether AlMgB14 has a band gap of 1.51 or 0.7 electron volts (eV)

Density Functional Theory is a method of approximating the electronic and material properties through quantum mechanics. DFT uses functionals to approximate the electron cloud and find solutions to the Schrodinger Equation through iteration. This allows the prediction of every atom in the unit cell. And knowing every atomic property allows every physical property to be deduced and understood. This study used the DFT software "**Quantum Espresso**" (QE) for all calculations.

Objectives

Approximating the Band Gap

- Knowing The band gap of a material is important for understanding the optical, electrical, and conductivity of that material.
- AlMgB14 Exhibits the properties of a semi-conductor. For semiconductors, a more complex method of DFT is needed to calculate the band gap. Hybrid Functionals are more complicated Functionals that can better approximate the Band Gap of a material at the major cost of computational resources.
- The standard AlMgB14 unit cell has 64 atoms. However, the true atomic structure is closer to **Al0.75B0.75B14** and has 62 atoms. Throughout the Boron orthorhombic structure, there are randomly missing Al and Mg atoms which contribute to its properties. To determine the properties accurately, the lowest energy and most stable state needs be found.

DFT Method

Configuring the Unit Cell

There was no available file of the unit cell that was available. That meant one had to be created. The file of a similar material, LiAlB14, was used and the lithium was replaced with magnesium to create the unit cell. UNC Charlotte's HPC supercomputer was used due to the size of the unit cell, often requiring days to complete a calculation.

Calculation Process

- **Optimization** calculations were the first calculation performed. These calculations "relax" or optimize the atomic positions of the atoms to find the lowest energy atomic configuration. The results were use in most subsequent calculations
- **Self-Consistent Field (SCF) and Non-Self-Consistent Field (NSCF)** calculations were the basis for all other calculations. SCF calculations approximate the lowest energy or ground state energy of the material. NSCF calculations calculate the energy of the bands.
- **BANDs and Density of State** calculations map the band interactions and band gaps throughout multiple **High Symmetry Points** in the Brillouin Zone (crystal lattice) and determine the number of states per energy value, respectively. AlMgB14 has 272 bands which made the calculations quite complex. BANDs and DOS calculations were performed before and after the Hybrid Functional calculations.
- **HSE06 Hybrid Functional** calculations were the primary calculation to determine the band gap energy. The complexity of the calculations due to the HF and large unit cell required 750 GB of RAM and up to 3 days to calculate.

SCF Energy Convergence Calculations Testing the 16 Different Al and Mg Configurations of the 62-Atom unit cell

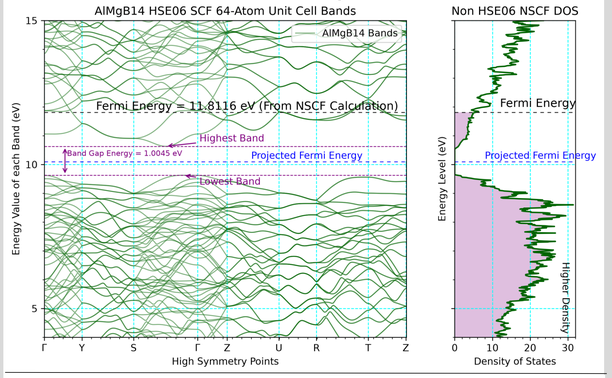
- The Unit Cells are grouped based on what Mg atoms are missing
- The 2nd column primarily of interest, displaying the energy of each unit cell. The energy of each cell is relatively the same, meaning each is similarly stable.

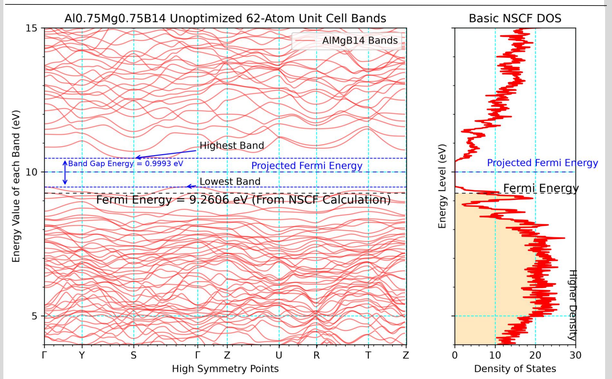
Confiuration	Total Energy (Ry)	TE Difference	Fermi Energy (eV)	Total Force (Ry/au)
Group 1	-1059.25179959		9.1483	0.1274185
Mg 0 Al 4	-1059.22802423		9.2606	0.1281580
Mg 0 Al 5	-1059.22802423	0.00E+00	9.2606	0.1281580
Mg 0 Al 6	-1059.27557495	4.76E-02	9.0360	0.1266790
Mg 0 Al 7	-1059.27557495	0.00E+00	9.0360	0.1266790
Group 2	-1059.25179959		9.1483	0.1274185
Mg 1 Al 4	-1059.27557495		9.0360	0.1266790
Mg 1 Al 5	-1059.27557495	0.00E+00	9.0360	0.1266790
Mg 1 Al 6	-1059.22802423	-4.76E-02	9.2606	0.1281580
Mg 1 Al 7	-1059.22802423	0.00E+00	9.2606	0.1281580
Group 3	-1059.25179959		9.1483	0.1274185
Mg 2 Al 4	-1059.27557495		9.0360	0.1266790
Mg 2 Al 5	-1059.27557495	0.00E+00	9.0360	0.1266790
Mg 2 Al 6	-1059.22802423	-4.76E-02	9.2606	0.1281580
Mg 2 Al 7	-1059.22802423	0.00E+00	9.2606	0.1281580
Group 4	-1059.25179958		9.1483	0.1274185
Mg 3 Al 4	-1059.22802423		9.2606	0.1281580
Mg 3 Al 5	-1059.22802420	-3.00E-08	9.2606	0.1281580
Mg 3 Al 6	-1059.27557495	4.76E-02	9.0360	0.1266790
Mg 3 Al 7	-1059.27557495	0.00E+00	9.0360	0.1266790
Total Avg	-1059.25179959		9.1483	0.1274185

Results

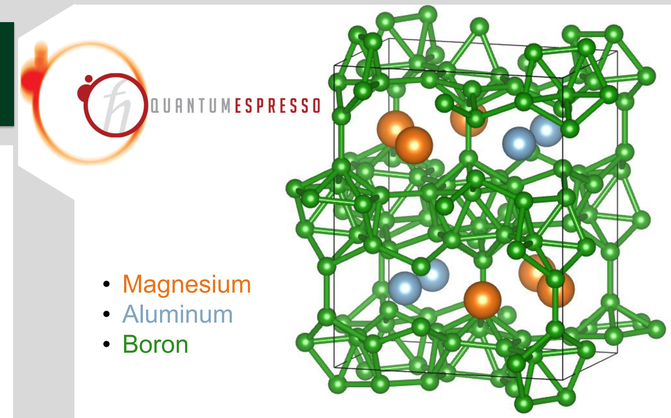
Atomic Stability and Approximated Band Gap

- There exists now a file of the AlMgB14 unit cell that will be uploaded to Materials Project for public use.
- All 16 Configurations of the 62-Atom Unit Cell were very stable and had near identical results from the SCF convergence calculations.
- The initial Band Gap calculated from normal SCF and the HSE06 SCF calculations was ~0.41 electron volts (eV) for both the 64 and 62 atom unit cells. However, SCF calculations are not very accurate for Band Gap calculations.
- The more accurate BANDs calculations for the 64 and 62 atom unit cell calculated the band gap as ~0.86 and ~0.9993 eV, respectively. The HSE06 calculation of the 64-atom unit cell estimated a 1.0045 eV Band Gap.
- The Fermi Energy ranged from ~11.260 – 9.143 eV for both the 64-and 62-unit cells. The true Fermi Energy predicted by the Bands and DOS calculations lies around 10 eV between the Lowest upper band and highest lower band.





BANDs (Left) and Density of States (Right) Calculations



The Atomic Structure of AlMgB14. The Basic Unit Cell Contains 64 Atoms.

Conclusions

Results and Limitations

AlMgB14 has a lot of potential applications. However, it is limited by the fact that its atomic properties are still unknown. The results of this study uncovered some interesting facts, Such as all 16 configurations of the 62-atom unit cell producing practically the same results, meaning every combination is stable. The Fermi Energy results stayed relatively constant for the respective unit cell, ~9.4 eV and ~11.2 eV for the 62 and 64-atom unit cells, respectively. And a file of the atomic unit cell now exists.

Since the HSE06 Non-Self Consistent Field could not be successfully finished, the Fermi Energy and Band Gap are likely inaccurate. Whether the Band Gap of AlMgB14 is 1.51 or 0.7 eV is still uncertain, but information on the true 62-atom Unit Cell has been achieved. There is still more work to be done with finishing Hybrid Functional calculations to determine every atomic property.

References

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