3rd International Conference on Scientific and Academic Research
December 25-26, 2023 : Konya, Turkey
AS-Proceedings
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First Principle Calculations of Structural, Electronic, and Optical Properties of MgAlO3: A Perovskite Oxide

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Abstract **–**. This paper presents a comprehensive exploration of the electronic structure and properties of magnesium aluminate (MgAlO3), a perovskite oxide with significant potential for diverse applications. Leveraging the power of Density Functional Theory (DFT), we delve into the fundamental aspects of MgAlO3, unravelling its electronic band structure, density of states, and defect properties. The electronic structure calculations offer valuable insights into the material's conductivity, optical characteristics, and bandgap, essential for understanding its suitability in electronic devices and other technological domains. Furthermore, the study investigates the stability of MgAlO3 under different conditions and explores the impact of defects, such as vacancies and dopants, on its properties. Through DFT simulations, we provide a detailed analysis of the interplay between electronic structure and defect engineering, offering a roadmap for tailoring MgAlO3 to specific applications. This research bridges the gap between theory and experiment, contributing to the broader understanding of perovskite oxides and facilitating the informed design of materials for future technological advancements. The investigation of the structural, electronic, and optical properties of the crystal structure was made using the Wien2k computer package program.

Keywords –DFT, MgAlO3, Electronic Structure, Perovskite Oxide, Optical Structure

I. INTRODUCTION

In the realm of materials science and condensed matter physics, the exploration of novel materials with unique properties and functionalities is at the forefront of research endeavors. Among these materials, perovskite oxides have garnered significant attention due to their diverse and tunable characteristics[1, 2]. One such compound, magnesium aluminate ($MgAlO_3$), exhibits promising features for various applications, ranging from electronic devices to catalysis [3-5]. In this paper, we delve into a comprehensive study of $MgAlO_3$ utilizing Density Functional Theory (DFT), a powerful computational approach that has revolutionized our understanding of the electronic structure and properties of materials.

1.1. Perovskite Oxides: A Brief Overview

Perovskite oxides, with their distinctive ABX3 crystal structure, have become a focal point in materials research due to their intriguing physical and chemical properties [6-8]. The general perovskite structure consists of an A-site cation, a B-site cation, and an oxygen framework. This arrangement allows for a myriad of compositions and, consequently, a wide range of functionalities. MgAlO3, with magnesium (Mg) occupying the A-site and aluminium (Al) at the B-site, represents a subset of perovskite oxides that holds promise for applications demanding tailored electronic and optical properties.

1.2. Significance of MgAlO3 in Materials Science

MgAlO3's significance lies in its potential applications in various technological domains [9]. For instance, its high thermal stability and excellent chemical resistance make it an attractive candidate for refractory materials. Furthermore, the compound's electronic properties make it a subject of interest in the development of electronic devices. Understanding the fundamental aspects of MgAlO3, such as its electronic structure and stability, is crucial for harnessing its full potential in practical applications.

1.3. Computational Framework: Density Functional Theory

Theoretical methods play a pivotal role in unraveling the intricacies of materials at the atomic and electronic levels. Among these methods, Density Functional Theory has emerged as a cornerstone for predicting and interpreting the properties of diverse materials [10-13]. DFT offers a balance between accuracy and computational efficiency, making it particularly well-suited for the study of complex systems like $MgAlO_3$ [14].

In the realm of DFT, the Schrödinger equation is solved by considering the electron density rather than the wave function, significantly reducing the computational burden [15]. The success of DFT lies in approximating the exchange-correlation functional, and various formulations, such as the widely used generalized gradient approximation (GGA) and hybrid functionals, have been employed to enhance accuracy [16].

1.4. Electronic Structure of MgAlO3: Insights from DFT

A fundamental aspect of $MgAlO_3$ that DFT allows us to explore is its electronic structure. By calculating the electronic band structure and density of states, we gain valuable insights into the behavior of electrons within the material. This information is critical for understanding its conductivity, optical properties, and potential as a semiconductor [4, 17].

Previous experimental studies have indicated that $MgAlO_3$ exhibits a wide bandgap, a characteristic often desirable in electronic materials. DFT calculations enable a deeper understanding of the bandgap, providing information about the nature of electronic transitions and the influence of defects on the electronic structure.

1.5. Stability and Defects in MgAlO3

Stability is a crucial factor determining the practical viability of materials. DFT allows us to assess the stability of $MgAlO_3$ under various conditions and identify potential phase transitions. Additionally, the investigation of defects, such as vacancies and dopants, is essential for tailoring the properties of $MgAlO_3$ to specific applications. Through DFT simulations, we can predict the impact of defects on the electronic structure and explore strategies to enhance or modify the material's characteristics.

In conclusion, the application of Density Functional Theory to $MgAlO_3$ provides a robust framework for unraveling its electronic structure, stability, and defect properties. By bridging theory and experiment, this computational approach enhances our understanding of perovskite oxides, paving the way for informed design and optimization of materials for diverse technological applications. This paper aims to contribute to the evolving landscape of materials science by providing a comprehensive exploration of $MgAlO_3$ through the lens of DFT.

II. Materials and Method

1. Computational details

The structural, electronic, and optic properties of the $MgAlO_3$ compound were performed by the full potential linearized augmented plane wave method (FP-LAPW) using the Wien2k code. The separation energy of valence and core states (Ecut) was chosen as -7 Ry. The convergence of the basis set was controlled by a cut-off parameter RmtKmax was selected as 7. The size of the largest vector in the charge density Fourier expansion (Gmax) was chosen as 12.

III. Results and Discussion

3.1. Structural Properties

$MgAlO_3$ compound is cubic with $Pm\bar{3}m$ (no. 5) space group (Fig. 1). The calculation was started with experimental data and calculated the total energy of the compound for various volumes around experimental data to find ground state properties. The calculated total energy depending on unit cell volume is given in Fig. 2.

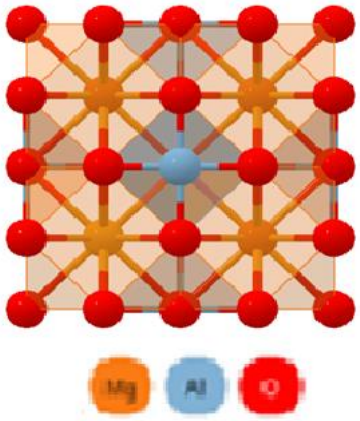

Fig 1. Unit cell of $MgAlO_3$

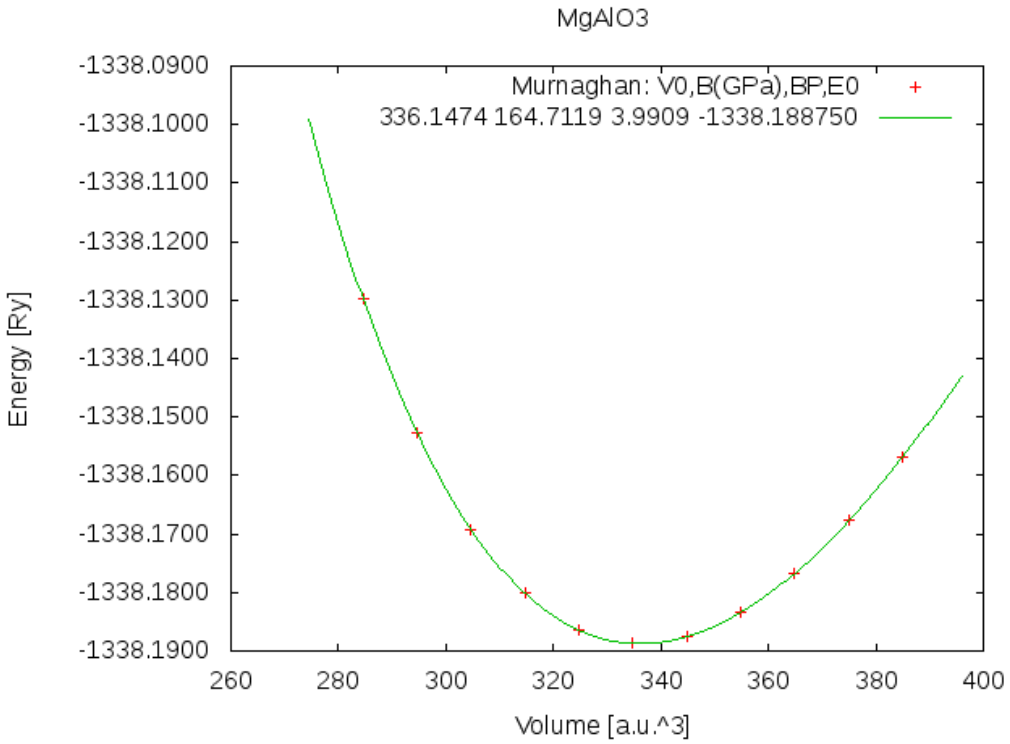

Fig 2. Calculated total energy versus unit cell volume of $MgAlO_3$ compound

The Calculated Structural Parameters of $MgAlO_3$ According to Murnaghan's equation, the calculated volume (V_0), bulk modulus (B_0), minimum energy (E), and derivative pressure (B_1) values are 336.1474 a.u. 3, 164.7119 GPa, -1338.18875Ry, and 3.9909 GPa, respectively.

3.2.Electronic properties

DOS (Figure 3), electronic band plot (Figure 4), and electron density plot (Figure 5) were drawn to determine the electronic properties of the compound.

The valence band maximum (VBM) is at M, the conduction band minimum (CBM) is at M point and $MgAlO_3$ has a direct gap (M–M).

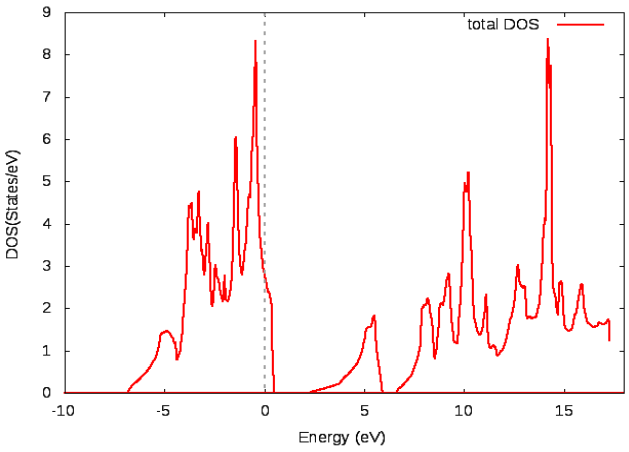

Fig 3. Calculated total DOS of $MgAlO_3$

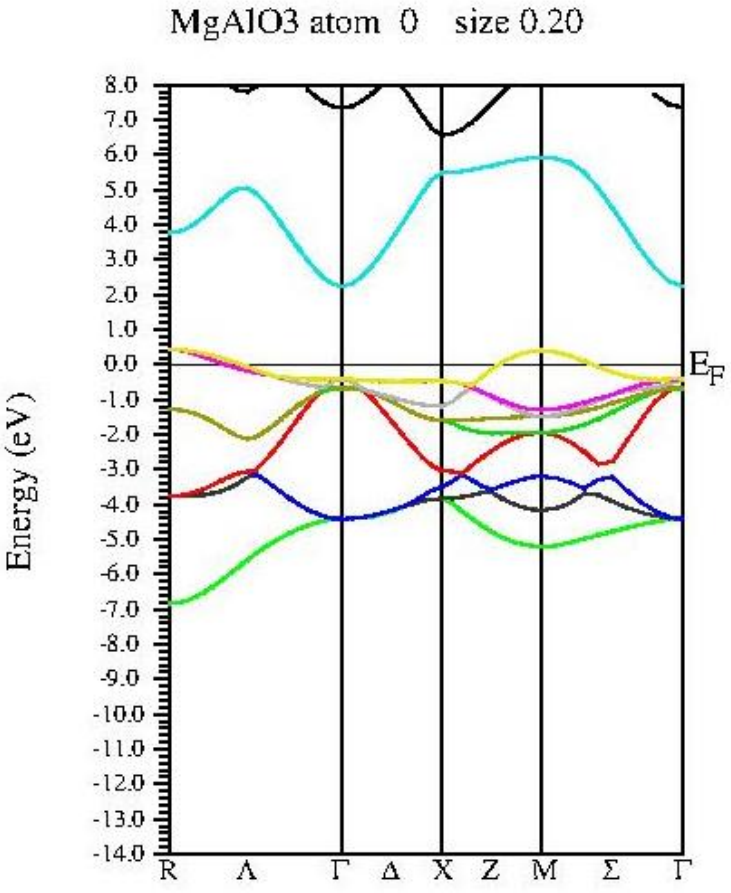

Fig 4. Electronic band plot of $MgAlO_3$

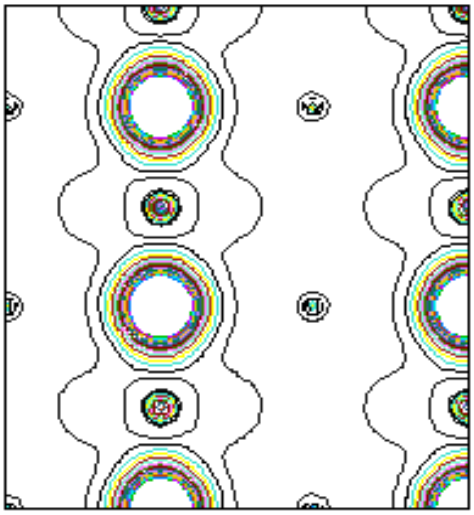

Fig 5. Electron density plot of $MgAlO_3$

3.1. Optical properties

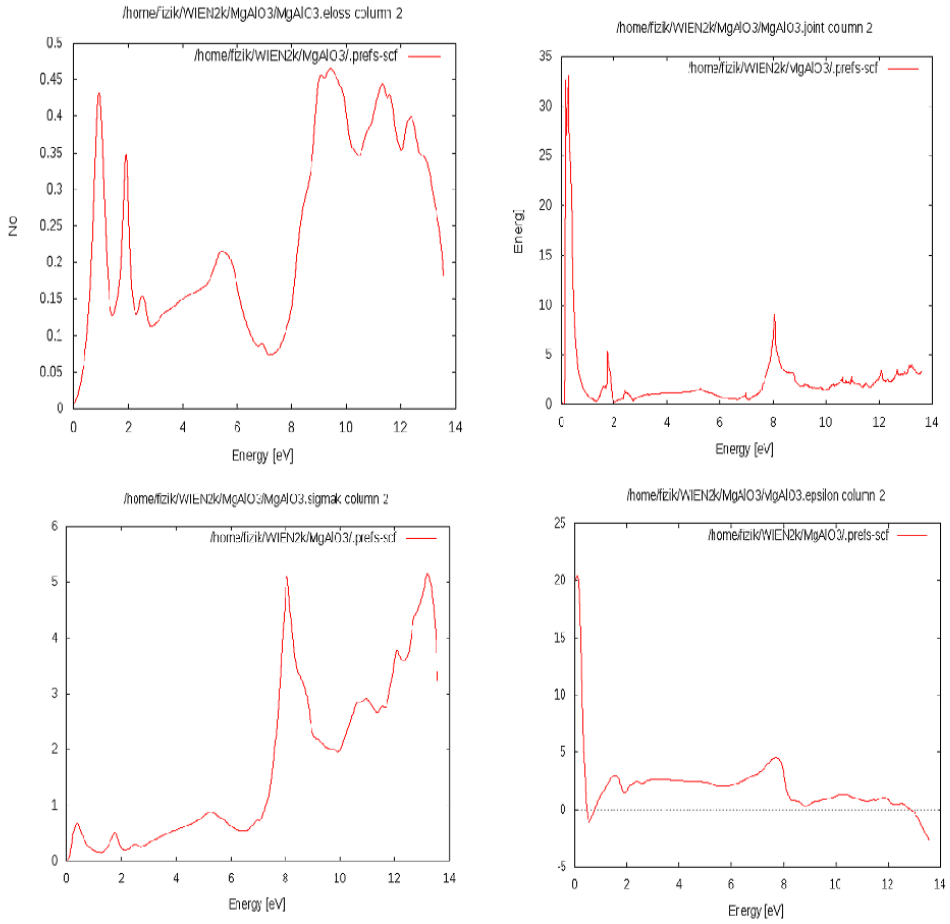

Fig 6. The optical properties of $MgAlO_3$

Fig. 6 shows the energies calculated for $MgAlO_3$

IV. CONCLUSION

The investigation of the structural, electronic, and optical properties of the crystal structure was made using the Wien2k computer package program. The calculation was started with experimental data and calculated the total energy of the compound for various volumes around experimental data to find ground state properties. The calculated total energy depending on unit cell volume is given graphically. Future studies could be carried out to reveal other phsical properties of the similar matarials.

REFERENCES

[1] X. Li *et al.*, "A-site perovskite oxides: an emerging functional material for electrocatalysis and photocatalysis," *Journal of materials chemistry A*, vol. 9, no. 11, pp. 6650-6670, 2021.

[2] S. Zhang, Z. Jia, B. Cheng, Z. Zhao, F. Lu, and G. Wu, "Recent progress of perovskite oxides and their hybrids for electromagnetic wave absorption: a mini-review," *Advanced Composites and Hybrid Materials*, vol. 5, no. 3, pp. 2440-2460, 2022.

[3] P. Liu, H. Li, and X. Zhou, "Clean synthesis of ethyl methyl carbonate using Mg-Al mixed oxide as catalyst," in *IOP Conference Series: Earth and Environmental Science*, 2021, vol. 687, no. 1: IOP Publishing, p. 012063.

[4] A. Zahoor, T. Mahmood, and M. I. Khan, "Mg-doped LaAlO3 structure: a theoretical investigation of indirect to direct bandgap and brittle to ductile transition," *Canadian Journal of Physics*, 2023.

[5] J. A. Muldoon and B. G. Harvey, "Bio-Based Cycloalkanes: The Missing Link to High-Performance Sustainable Jet Fuels," *ChemSusChem*, vol. 13, no. 22, pp. 5777-5807, 2020.

[6] R. H. Mitchell, M. D. Welch, and A. R. Chakhmouradian, "Nomenclature of the perovskite supergroup: A hierarchical system of classification based on crystal structure and composition," *Mineralogical Magazine*, vol. 81, no. 3, pp. 411-461, 2017.

[7] H. A. Evans, Y. Wu, R. Seshadri, and A. K. Cheetham, "Perovskite-related ReO3-type structures," *Nature Reviews Materials*, vol. 5, no. 3, pp. 196-213, 2020.

[8] F. K. Naqvi, Y. Khan, S. Beg, and A. Ahmad, "Types of Perovskite Materials," *Perovskite Materials for Energy and Environmental Applications*, pp. 241-255, 2022.

[9] B. Torres and M. Lieblich, "Room and high temperature tensile behaviour of a P/M 2124/MoSi 2 composite at different heat treatment conditions," *Journal of materials science*, vol. 41, pp. 3493-3500, 2006.

[10] A. S. Rosen, J. M. Notestein, and R. Q. Snurr, "Identifying promising metal–organic frameworks for heterogeneous catalysis via high-throughput periodic density functional theory," *Journal of computational chemistry*, vol. 40, no. 12, pp. 1305-1318, 2019.

[11] P. Blaha, "WIEN2k, an augmented plane wave plus local orbital package for the electronic structure of solids," 2021.

[12] P. Blaha, K. Schwarz, F. Tran, R. Laskowski, G. K. Madsen, and L. D. Marks, "WIEN2k: An APW+ lo program for calculating the properties of solids," *The Journal of chemical physics*, vol. 152, no. 7, 2020.

[13] E. Bosoni *et al.*, "How to verify the precision of density-functional-theory implementations via reproducible and universal workflows," *Nature Reviews Physics*, pp. 1-14, 2023.

[14] R. J. Maurer *et al.*, "Advances in density-functional calculations for materials modeling," *Annual Review of Materials Research*, vol. 49, pp. 1-30, 2019.

[15] D. S. Sholl and J. A. Steckel, *Density functional theory: a practical introduction*. John Wiley & Sons, 2022.

[16] A. Patra, B. Patra, L. A. Constantin, and P. Samal, "Electronic band structure of layers within meta generalized gradient approximation of density functionals," *Physical Review B*, vol. 102, no. 4, p. 045135, 2020.

[17] D. Peng, Y. Zhang, Y. Zhang, and X. Huang, "Valence Band Edge Engineering of Mixed Metal Oxides Photocatalysts Derived from Transition Metal Intercalated Layered Double Hydroxide Towards Selective Oxidation of Cyclohexane Under Visible Light," *Available at SSRN 4110640*.