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Original Research Article

A Theoretical Investigation for Electronics Structure of $Mg(Bio_2)_2$ Semiconductor Using First Principle Approach

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ABSTRACT

The Mg(BiO2)2 is the orthorhombic crystal system acting as semiconductor in electric devices. To evaluate electronic band structures, the total density of state (TDOS) and the partial density of state (PDOS), Generalized Gradient Approximation (GGA) based on the Perdew–Burke–Ernzerhof (PBE0) was used for Mg(BiO2)2. The band gap was recorded at 0.959 eV, which is supported by a good semiconductor. The density of states and partial density of states were simulated for evaluating the nature of 5s, 4d for Mg, 6s, 4f, 5d, 6p for Bi and 2s, 2p for O atom for Mg(BiO2)2 to explain the transition of the electron due to hybridization. From the PDOS, it was illustrated that the d orbital of Bi atom responses for conducting the electronic holes.

Keywords: Electronic band structures, TDOS, PDOS, GGA and $Mg(BiO_2)_2$.

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INTRODUCTION

$Mg(BiO_2)_2$, one of the metal borates, is one of the most critical technical ceramics owing to its impressive properties, such as high heat resistance and corrosion resistance, superb mechanical strength, superb insulation, and a high coefficient of elasticity [1; 2]. With the development of the global semiconductor industry, semiconductor materials are a fundamental element for the information society high-tech industry, and the 21st century has become the big data era [3; 4; 5]. High-speed computing, large-capacity data communication, storage, processing, electronic devices are very important for the development of national economy and national security. It is one of the basic and supporting materials required for the production of electronic circuits such as large circuits, flat display devices, compound semiconductor devices, solar cells, and optical fibers and with this, the use of semiconductors is increasing day by day, the role of semiconductors is in the field of discovering new advanced technologies. Without downstream IC, LCD / LED, BJT, MOSFET, transistor, resistor, and photovoltaic solar power can not be produced without semiconductors [6]. The semiconductor device is just a name insulating a small band gap. A semiconductor material changes its electronic properties in a controlled way. Transistors, lasers and solar cells, new devices, discovering new devices, and existing materials are considered as important media for advanced content science research due to their applications in the computer and photovoltaic industry. This prevents the electrons of the semiconductor material from being transferred from one atom to another. Germanium silicon, carbon, selenium, mixed acid water, etc. are most commonly used as semiconductors, while germanium, silicon, semiconductor atomic structure is a crystalline shape [7]. Besides germanium, silicon, bismuth, iron, strontium are widely used as semiconductor materials in the present time in the different advanced electronic devices due to their good conductivity. Moreover, the crystal of germanium, silicon, bismuth, iron, strontium, and antimony oxide have been established as a semiconductor because of its thermal capacity, and the Forbidden Energy Gap remains high despite its outer cell having the same balance electrons [8]. Its current conductivity works much higher and at higher temperatures than other semiconductors. Due to these specifications, semiconductor electronics requirements of $Mg(BiO_2)_2$ are high.

Among the various kinds of metal borates, like magnesium borate $Mg(BiO_2)_2$ crystal has been considered to have promise as a reinforcing component in composite material applications due to its excellent mechanical properties, attractive thermal properties[9], thermo-luminescent properties [10; 11], and good antiwar behavior [12]. In recent years, there has been a great deal of research in the use of $Mg(BiO_2)_2$ to reinforce Mg and Al matrix composites, which has had considerable success. It should be noted that the excellent mechanical properties of the $Mg(BiO_2)_2$ also imply their promise as a reinforcing additive for polymers. This kind of polyester can be biologically synthesized from bio-renewable feedstock and is generally biodegradable and biocompatible [13; 14; 15]. However, the brittle nature of the Polyhydroxyalkanoates(PHA) polymers has hindered their development in practical applications. Reinforcing PHA polymers by the incorporation of $Mg(BiO_2)_2$ nanowires provides the possibility to obtain composite materials with high mechanical strength.

The electronic structure calculations were performed using both the full-potential linearized augmented plane wave method and the ultrasoft pseudo-potential plane wave method, respectively. Within the former method, no shape approximation is used either for the potential or for the electronic charge density while in the latter method. Having a vast application in the area of polymer science, electronic devices, and photocatalysts, there was a large lack of theoretical profile and computational literacy of $Mg(BiO_2)_2$. In view of this purpose, we make use of the CASTEP program package within the generalized gradient approximation of Perdew–Burke–Ernzerhof for the exchange-correlation energy to regenerate the band structure, density of states and optical properties while the advangates of this method is to save time consumption, employee, no decay of equipments and experimental cost with environment sustainability. Finally, we have developed a theoretical investigation in this study with fine accuracy evidence.

COMPUTATIONAL METHODS

The method of GGA with PBE0 was optimized for CASTEP code from the material studio to calculate the band gap and density of the state [16]. In this condition, the band gap and density of state were calculated using the cut off at 510, and k point at 2×2×4 with non-conserving pseudopotentials. Then the optical properties were similar way simulated for calculation of refractive index, reflectivity, absorption, conductivity, and loss function. In additionally, the geometric optimization was achieved, and the convergence criterion for the force between atoms

was 3×10^{-6} eV/˚A, the maximum displacement was 1×10^{-3}˚A, and the total energy and the maximal stress were 1×10^{-5} eV/atom and 5×10^{-2} GPa, respectively. In a similar way, Ge was doped replacing Bi by 8.3% using building option, and supercell option and finally, all the above properties using a similar option was simulated.

Result And Discussion

Optimized Structure

The lattice parameters value are a = 3.275 Å b = 5.869.Å, c = 11.184 Å and angels between them as α= 90.000° β= 90.000°A°, γ= 106.203° A°. The monoclinic $Mg(BiO_2)_2$ crystal and the space group is Hermanna Mauguin Cmcm orthorhombic crystal system, point group mmm, hall -C 2c 2, density 8.14 g/cm^{3}shown in figure 1.

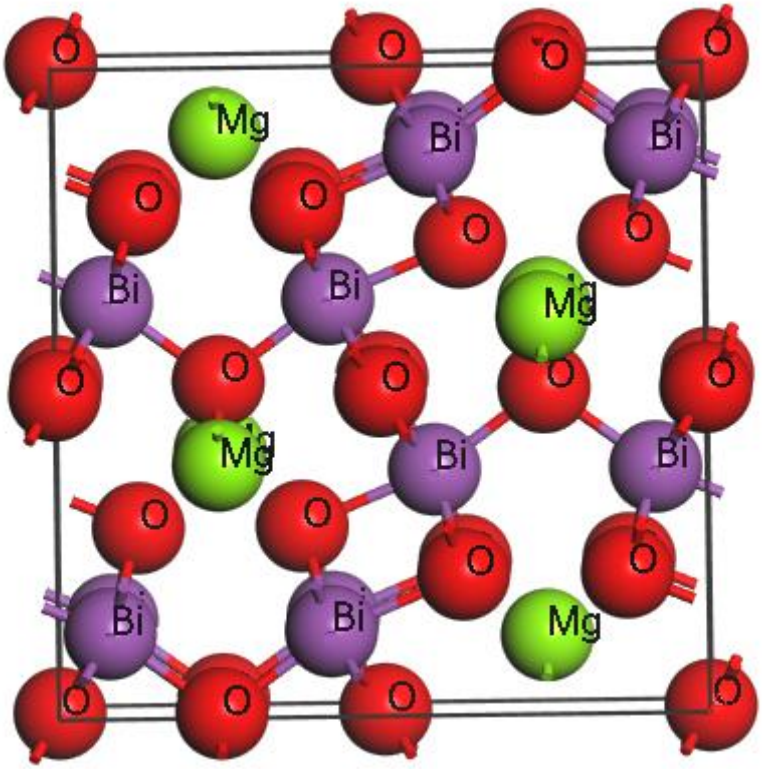

Figure 1: $Mg(BiO_2)_2$ structure

Electronic Structure

The band structures for $Mg(BiO_2)_2$ are given in figures. In the absence of Mg, such as in Mg $(BiO_2)_2$, the bottom of the Bi-d band at the G point lies below the top of the Mg p-band at the Y or Z point, making it a metal. However, strongly perturb with the Bi-orbitals. This band at the G point in $Mg(BiO_2)$, gets pushed sufficiently up and now lies above the Fermi energy. This opens up an energy gap and makes these systems indirect narrow gap semiconductors. To determine the electronic band structure of Mg (BiO_2), the Fermi energy level was set at zero. From figure 2, it was found that the minimum of conduction bands (MCB) was obtained at the G symmetry point, whereas the maximum of valance bands (MVB) was also linked in G symmetry points. As both MCB and MVB are at point G symmetry, it is called a direct band gap, and it is calculated by 0.959 eV. From this figure 2, it can be said that both upper and lower parts of the conduction band are well dispersive in the near Z, and Y symmetry points than G and S symmetry point. On the other hand, the upper level of a valance band near the Y symmetry point is equally dispersive, but the lower part doesn't disperse. In general, a lower carrier effective mass corresponds to higher carrier mobility.

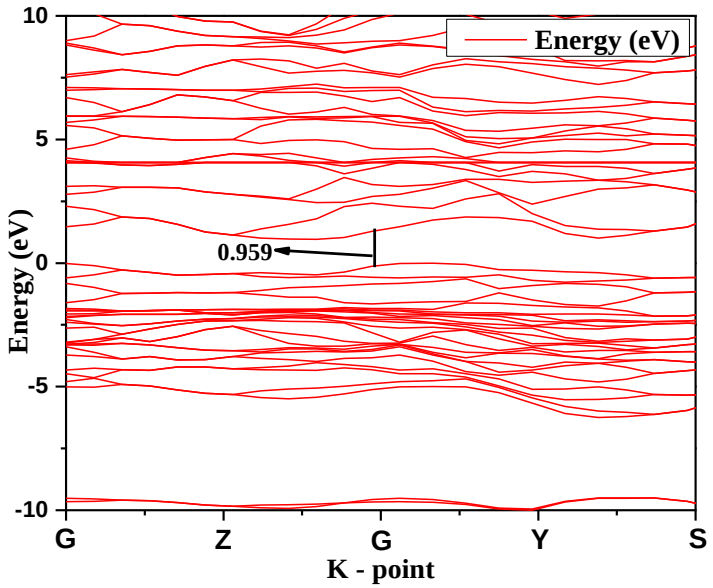

Figure 2: Electronic structure

The Density Of State And Partial Density Of State

A new method is used to derive an accurate but simple formula for the state density for fixed numbers of particles and holes in the uniform spacing model. The calculation is extended to the case where two kinds of particles are present. The results are compared with exact numerical calculations. Direct numerical calculation of particle-hole state densities, asymptotic summation of the approximate formula, and angular momentum distribution of states are discussed in the appendices. The density of states indicates the nature of electronic band structures and the splitting of an orbital. The density of total states (DOS) of Mg, Bi, and O elements for $Mg(BiO_2)$, crystals were calculated by PBE0 with GGA. From figure 3, it was found that the valence bands are mainly occupied by 3s, 3p for Mg, 6s 4d, 6p for Bi and 2s, 2p for O elements. Meanwhile, above the Fermi level, the conduction bands are composed of Mg in 3s, 3p orbital. As shown in figure 3, the bands just below the Fermi level and above the Fermi level, it is noted that total density of state for $Mg(BiO_2)$ and it is evaluated that the DOS for s, p, d, and sum for is more delocalized than showing in fig 3(a), 3(b), 3(c), 3(d), and 3(e), higher delocalizing the d orbital.

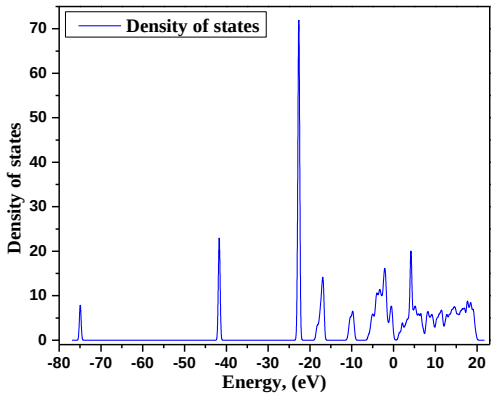

Figure 3(a): Total DOS

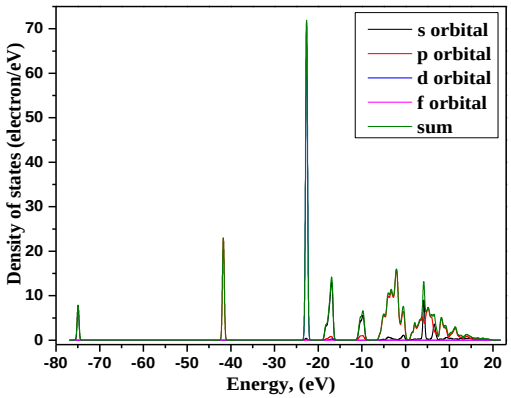

Figure 3(b): PDOS

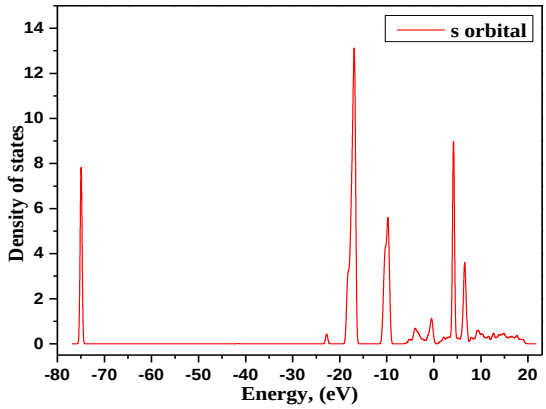

Figure 3(c): DOS of s orbital

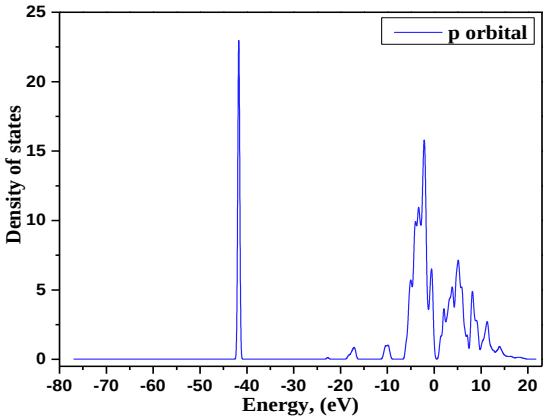

Figure 3(d): DOS of a p orbital

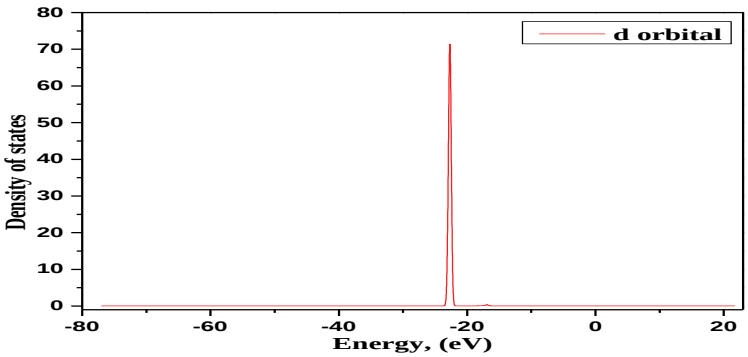

Figure 3(e): DOS of d orbital

Conclusion

This observation and the calculated band gaps for binary and ternary semiconductors relevant to photovoltaics constitute the main results of this paper, $Mg(BiO_2)_2$ is a semiconductor. In our calculation, we have used the generalized gradient approximation (GGA) on the Perdew–Burke–Ernzerhof (PBE0) within the method to study the electronic structures of $Mg(BiO_2)_2$ crystal. From the electronic structure, the band gap was 0.959, and the delocalization was also enlarged. Dramatically better band gaps for the binary and ternary semiconductor compounds that are of interest in photovoltaics and thermoelectric.

Reference

[1] F. Qin, G. Li, R. Wang, J. Wu, H. Sun, R. Chen, *Chem. A. Europ. J.,* 18, 16491(2012).

[2] A. Etogo, E. Hu, C. Zhou, Y. Zhong, Y. Hu, Z. Hong, *J. Mater. Chem. A.,* 3, 22413 (2015).

[3] V. Hegde, A. Wagh, H. Hegde, C.D. Vishwanath, S.D. Kamath, *Appl. Phys. A.,* 123, 302 (2017).

[4] A. Khanna, S. Bhatti, K. Singh, K. Thind, *Nucl. Instrum. Meth. B.,* 114, 217 (1996).

[5] Z. Xuejia, Development and application of boron and borate Inorganic Chemicals Industry (2005).

[6] V.G. Alessandro, Pierluigi; Daliento, Santolo, *IEEE. J. Photovolt.,* 4, 405 (2013).

[7] S.A.W. Dayeh, Jian; Li, Nan; Huang, Jian Yu; Gin, Aaron V; Picraux, S Thomas, *Nano. Lett.,* 11, 4200 (2011).

[8] V.T. Agekyan, *Phys. Stat. solid.,* (A) 43, 11 (1977).

[9] C.W. Nyambo, Charles A, *Polym. Degrad. Stab.,* 94, 506 (2009).

[10] A. Durin-France, L. Ferry, J.M. Lopez Cuesta, A. Crespy, *Polym. Int.,* 49, 1101(2000).

[11] R. Ma, Y. Bando, D. Golberg, T. Sato, *Angew. Chem. Int. Ed. Engl.,* 42, 1836 (2003).

[12] S. C.W. Zhang, Bo-Kang; Cai, Qi-Zhou; Wang, Li-shi, *Trans. Nonferrous Met. Soc. China.,* 13, 83(2003).

[13] S.V. Dorozhkin, *Acta. Biomater.,* 10, 2919 (2014).

[14] I. Cacciotti, *J. Mater. Sci.,* 52, 8812 (2017).

[15] M. A. Soriano-Ursua, B. C. Das, J. G. Trujillo-Ferrara, *Expert. Opin. Ther. Pat.,* 485 (2014).

[16] J.P.B. Perdew, Kieron; Ernzerhof, Matthias, *Phys. Rev. lett.,* 77, 3865 (1996).

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