STUDY OF STRUCTURAL AND ELECTRONIC PROPERTIES OF CsMgCl₃ COMPOUND

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In this report, we have investigated the CsMgCl₃ compound with the help of the WIEN2K software package. The structural and electronic properties are performed using the full potential augmented plane wave (FP-LAPW) method with the generalised gradient approximation (GGA) approximation as exchange correlation potentials. We used the Birch-Murnaghan equation (BME) to find the structural properties of the material. These include the lattice parameter, the bulk modulus, the first derivative of the bulk modulus, the minimum energy, and the volume. The structural properties match up with the experimental data. Electronic properties in terms of the band structure (BS) and total and partial density of state (T-DOS and P-DOS) profiles of CsMgCl₃ using GGA potentials exhibit an indirect wide energy band gap of 5.35 eV. All these properties show that the CsMgCl₃ compound is used as a perovskite in solar cells.
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1. INTRODUCTION

The extraction of power from the most cost-effective sources, with the most efficient techniques, has garnered considerable attention among materials scientists. Hence, to ascertain the position of products in actual applications, it is imperative to define the operational characteristics of these gadgets. The utilisation of solar energy and the recovery of lost heat have significant promise. In recent times, there has been a significant surge in research pertaining to materials and compounds associated with photovoltaic technology and energy conversion applications. This surge can be attributed to the escalating impact of climate change and its detrimental consequences on the environment. According to this perspective, several halide perovskite compounds, both organic and inorganic in nature, have demonstrated significant promise as materials for photovoltaic applications such as solar cells. These compounds exhibit characteristics such as high-power conversion efficiency, high carrier mobility, and other desirable properties [1-8]. Collectively, these materials have been recognised for their exceptional capabilities in electrical, optoelectronic, and thermoelectric transportation applications [9–12]. The organic-inorganic hybrid halide perovskite CH₃NH₃PbI₃ has garnered significant attention from researchers because to its notable characteristics, such as extensive absorption, high mobility, and several advantageous thermoelectric and optoelectronic properties [11, 13-16]. However, certain limits have been noticed, including the fact that led increases toxicity, which is not desirable from an environmental perspective [17]. Furthermore, it has been observed that the organic component undergoes decomposition, resulting in the release of detrimental chemicals [18]. To achieve the synthesis of lead-free perovskite compounds, alternative metal atoms such as Sn or Ge, with similar oxidation states, were substituted for the Pb atom. This substitution led to the development of certain pure inorganic and hybrid organic-inorganic compounds [19-21]. However, the substitutions indicate that lead-free compounds exhibit somewhat lower energy conversion efficiency and a lower figure of merit (ZT), which is a measure of the effectiveness of a thermoelectric material [22-23]. Consequently, there is a pressing need to conduct further research on alternative perovskite halides. Extensive research has been conducted on pure inorganic halide perovskite compounds due to the thermal decomposition of the organic component in hybrid perovskites at elevated temperatures [18]. Various studies have been conducted on compounds with diverse structural configurations, primarily focusing on their attributes through computational methods. The typical representation of their structure is ABX₃, wherein A and B are typically metals derived from main group elements, and X represents halides, specifically atoms of chlorine (Cl), bromine (Br), and iodine (I). Several lead-free halide perovskites have been identified, including CsGeX₃, CsSnX₃, TlGeX₃, TlSnI₃, CsMgBr₃, and others [24–28]. We have conducted research on hazardous inorganic perovskite compounds, specifically CsMgCl₃, which exhibit similarities to the compounds. CsMgI₃ has been omitted from consideration due to the findings of Ray et al, who determined that its cubic structure is not energetically possible as indicated by its positive formation energy [10]. Several experimental studies have been undertaken on CsMgX₃ compounds, focusing on their synthesis and structural analysis. These compounds have a

hexagonal lattice structure and are classified as non-perovskite compounds [29-31]. In a recent publication, Kaewmeechai et al., conducted a computational analysis on the structural and electrical characteristics of $CsMgBr_3$ in its three distinct phases [28]. However, it is important to note that there is a lack of comprehensive research conducted on the perovskite $CsMgX_3$ compounds. The past research findings indicate that halide perovskites belonging to the ABX_3 class can be found in cubic, tetragonal, and orthorhombic crystal systems. In light of the significant value associated with halide perovskites, there is a clear need to conduct a methodical and accurate examination of compounds belonging to the ABX_3 category. Such an inquiry holds great potential for enhancing our understanding in this field. Although there is a lack of comprehensive theoretical details about the potential optical applications of a computational approach, the existing body of experimental literature predominantly emphasises optical applications. In addition, there is a lack of research that elucidates the impact of halogen ion replacement on the optical and thermoelectric properties of $CsMgCl_3$. This study focuses only on the cubic phases of $CsMgCl_3$, examining their structural, and electronic properties using the GGA functional. These properties have not been previously investigated.

2. COMPUTATIONAL METHODOLOGIES

The simulations of $CsMgCl_3$ halide perovskites were conducted using the WIEN2K code, employing the self-consistent full-potential linearized augmented plane wave (FP-LAPW) approach. This method was integrated into the code [32-33]. The structural optimisation was performed using the PBE-GGA (Perdew-Burke-Ernzerhof generalised gradient approximation) exchange functional [34]. To accurately calculate the electronic characteristics, we employed the GGA exchange correlation functional [35], which yielded improved outcomes. The implementation of this technique necessitates the partitioning of the crystal structure into muffin-tin (MT) spheres that encompass the atomic sites and the interstitial regions located at the periphery of these spheres. In order to achieve Eigen-value convergence, a value of 8.0 is chosen for Rmt*Kmax, where Rmt represents the muffin tin radius. It is typically selected to be sufficiently big to prevent any overlap between the MT spheres. Kmax, on the other hand, refers to the maximum value of the reciprocal lattice vectors and is of utmost importance. The expansion of angular momentum is carried out by performing calculations using a k-mesh consisting of 15×15×15 k points, which allows for the integration of the irreducible Brillouin zone. The number of k-points in the Brillouin zone has been augmented to 2456, as the attributes under consideration exhibit a strong reliance on the higher density of k-points. The accompanying section fully presents all the equations involved in the computation of these properties.

3. RESULTS
3.1. Structural Properties

As previously stated, we have considered the cubic arrangement of the perovskite compounds under investigation and conducted structural optimisations. The fully relaxed structure is depicted in Figure 1. The Wyckoff positions for Cs and Mg atoms are designated as 1a (0, 0, 0) and 1b (0.5, 0.5, 0.5) respectively. Conversely, the halide ions (Cl) are situated in the 3c positions, namely (0, 0.5, 0.5), (0.5, 0, 0.5), and (0.5, 0.5, 0). The compounds with cubic structure are classified under the Pm3m space group.
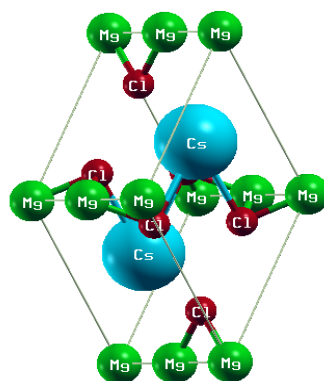

Figure 1. Unit cell structure of $CsMgCl_3$ generated by VESTA

The lattice parameters and other physical attributes, as presented in Table 1, were determined through volume optimisation using the Birch-Murnaghan equation of state, written as follows [36]:

$$E_{total} = E_0(V) + \frac{B_0 V_0}{B_0'(B_0' - 1)}\left[B_0\left(1 - \frac{V_0}{V}\right) + \left(\frac{V_0}{V}\right)^{B_0'} - 1\right]. \tag{1}$$

The equation was utilised to provide a graphical representation of the relationship between energy and volume, which is depicted in Figure 2. By analysing these plots, we can determine the minimal energy of the compounds in their ground state, as well as the corresponding optimum volumes. This analysis is conducted using the PBE-GGA method.

According to the data presented in Table 1, it is evident that the lattice constants for $CsMgCl_3$ is 7.29 Å, respectively. Notably, the latter value closely corresponds to a previously reported finding [28]. The observed bulk modulus and its pressure derivative for these compounds indicate that their values are not significantly like those of metals. This suggests that these compounds possess a modest level of compressibility.

Table 1. Calculated lattice constants (a_0), Min. cell volume (V_0), Ground state energy (E_o), Bulk modulus (B_0) and Pressure Derivative of bulk modulus (B_P), Band gap (E_g) and Fermi energy (E_F) of cubic $CsMgCl_3$.

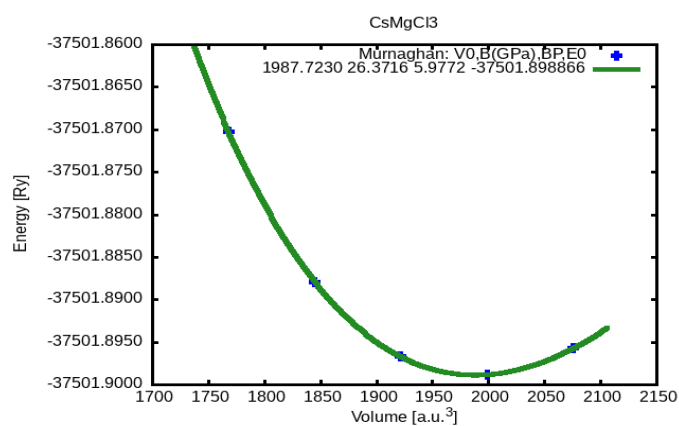| Parameters	CsMgCl₃	Experimental
Lattice parameter (Å)	7.292908648	5.178 [28]
Min. Volume (a. u)³	1987.7230	------
Bulk Modulus B (GPa)	26.3716	------
Pressure derivative B_P(GPa)	5.9772	------
Minimum energy E_o (Ryd)	-37501.898866	------
Bandgap(eV)	5.35	6.35 [37]
Fermi energy (E_F)	0.02259	-------

Figure 2. Variation of total energy with volume of $CsMgCl_3$ compound

3.2. Electronic Properties

To examine the electronic properties of these compounds, we have conducted calculations on their band structures using the PBE-GGA exchange correlation functionals. The results are presented in Figures 3(a-b).
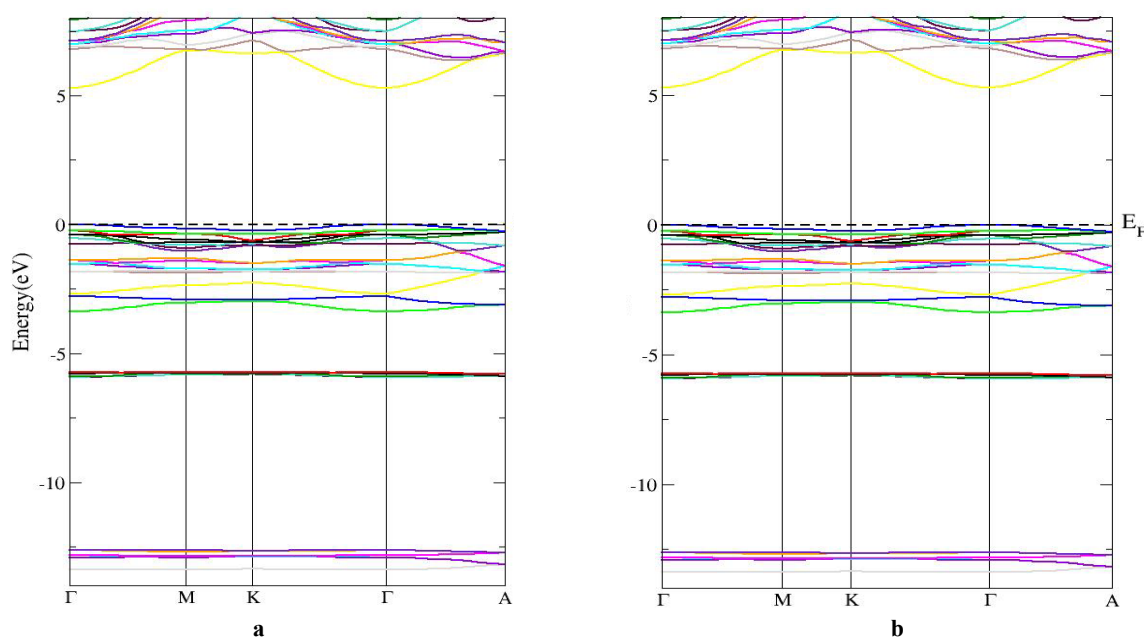

Figure 3. Electronic band structures of (a) $CsMgCl_3$ for spin up, (b) $CsMgCl_3$ for spin down, using GGA approach.

Various research in the field of density functional theory (DFT) have noted that the utilisation of exchange functionals can occasionally present challenges when attempting to accurately determine band gaps. The PBE-GGA functional has been found to significantly underestimate the band gaps of different materials and compounds due to a

self-interaction mistake. This issue could be addressed by utilising alternative methodologies, a highly effective approach that is extensively employed in DFT calculations for determining the electronic structure and various properties of compounds such as perovskites and Heusler alloys. In our investigation, we have calculated band gap for $CsMgCl_3$ compound by the utilisation of the generalised gradient approximation (GGA) technique with high symmetry k-points within the Brillouin zone is $\Gamma \rightarrow M \rightarrow K \rightarrow \Gamma \rightarrow A$, which is utilised for the computation of electronic structures. To begin with, the band structures of $CsMgCl_3$, as depicted in Figure 3(a-b), indicate that it exhibits characteristics of indirect wideband gap materials.
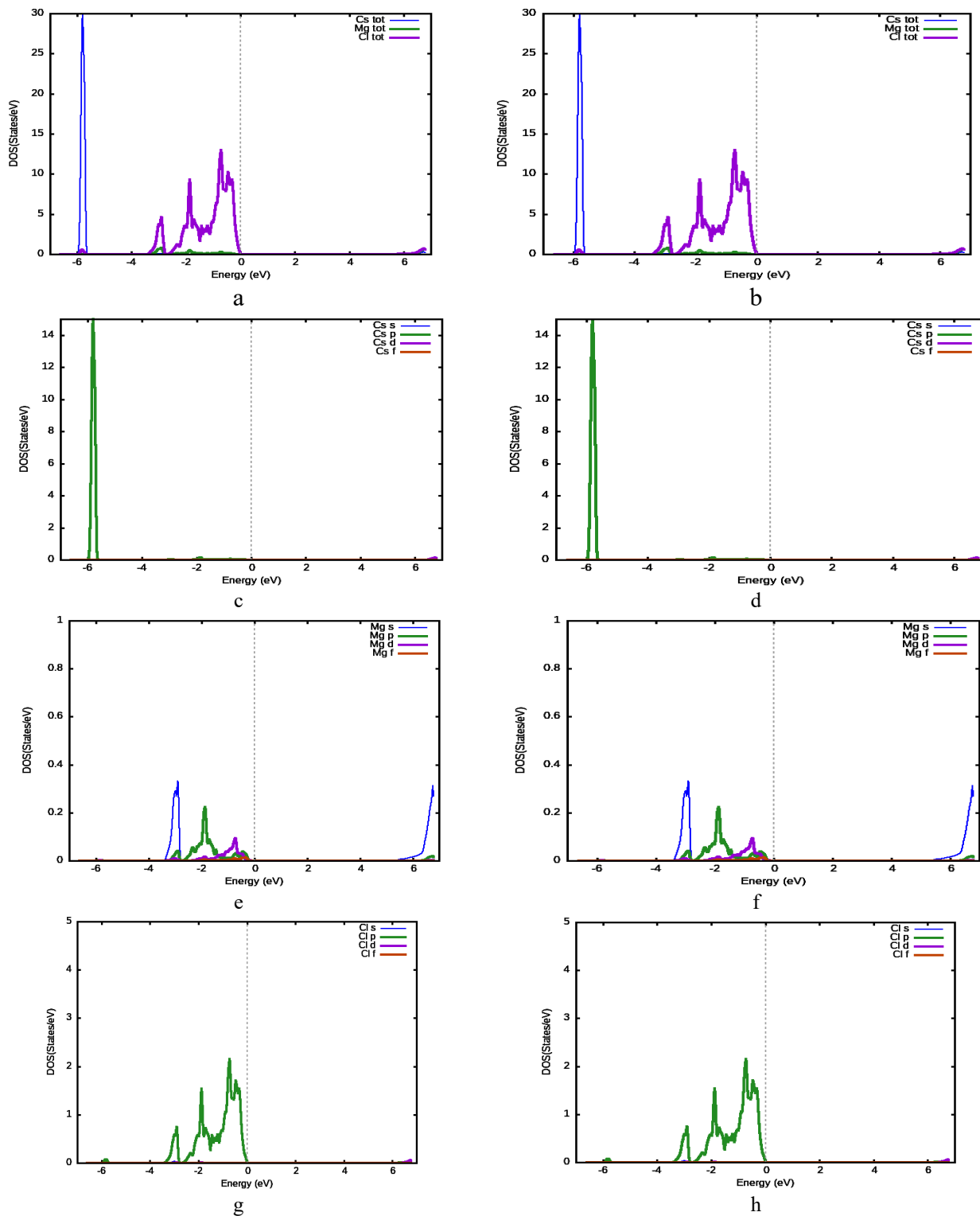

Figure 4. Total density of states of (a) $CsMgCl_3$ in spin-up, (b) $CsMgCl_3$ in spin-down and partial density of states of (c) Cs (s, p, d and f state) in spin-up, (d) Cs (s, p, d and f state) in spin-down, (e) Mg (s, p, d and f state) in spin-up, (f) Mg (s, p, d and f state) in spin-down, (g) Cl_3 (s, p, d and f state) in spin-up, (h) Cl_3 (s, p, d and f state) in spin-down

The conduction band minimum (CBM) is located at the Γ point, whereas the valence band maximum (VBM) is situated at the M point, resulting in the formation of an indirect gap. Nevertheless, a band gap of these compound found is 5.35 eV has been attained using GGA. It is important to note that the characteristics of the conduction and valence bands (CB and VB) are consistent in both cases. Additionally, it has been observed that the bands in the valence band (VB) are located at the Fermi level and exhibit a relatively low curvature at high-symmetry points. The presence of flat bands in a system suggests the existence of high effective masses, which can significantly influence the efficiency of transport properties. The findings of our study regarding the energy band gap of CsMgCl$_3$, as determined using the GGA potential, demonstrate a proximity to the experimental value of 8.5 eV. Furthermore, the bandgaps of our theoretical models exhibit a high level of concordance with the perovskite structures described. The electronic band profiles of these compounds demonstrate their characteristic as wide band gap semiconductors when analysed using the PBE-GGA potential. However, under ambient conditions, they exhibit insulating behaviour when assessed using the GGA method.

Another electronic property calculated such as the total density of states (TDOS) and partial density of states (PDOS) were calculated for these compounds using the GGA potential in order to gain a better understanding of the specific atoms and their orbitals that contribute to the band structure curves. This potential was chosen due to its ability to produce an enhanced band gap. The TDOS plot of CsMgCl$_3$, as illustrated in Figure 4(a-h), indicates that the primary contribution to the density of states (DOS) in the valence band (VB) arises from the halogen atom (Cl) located at the Fermi level edges. This halogen atom is also accountable for the presence of flat bands at the VB band boundaries. A notable increase in the energy levels of a Cs atom is observed at higher energy values, approximately 5 eV. This phenomenon is associated with the presence of degenerate bands in the valence band that exhibit a flat energy profile near this energy range. The appearance of states in the conduction band (CB) at higher energy levels, around 6.3 eV, can be attributed to the energy gap resulting from the lack of density of states (DOS) in the CB region at the Fermi level (E$_F$) up to approximately 6.3 eV. The study reveals a comparable contribution of the Cl and Cs atomic states in the CB system. The participation of the magnesium (Mg) atom is nearly negligible in the valence band (VB) and fairly evident in the conduction band (CB).

The relationship between specific orbitals of the atoms in the electronic structures of perovskite compounds is elucidated by the PDOS plot depicted in Figure 4 (c-h). The analysis of Fig. 4(a) and (b) reveals that the prominent peaks observed in the valence band (VB) can be attributed mostly to the density of states (DOS) originating from the p-orbitals of Cl atom in the vicinity of the Fermi energy (E$_F$). Additionally, a narrow peak corresponding to the energy states of p-orbitals of Cs atoms at higher energies is also observed. Additionally, we observe a negligible contribution from the s and p-orbitals of magnesium atoms. In the context of the chemical bond, the participation of halogen atoms experiences a significant decrease. Small peaks of states for magnesium (Mg) atoms, specifically in their s and p-orbitals, are observed at higher energy levels within the conduction band. The occurrence of density of states (DOS) in Cs atoms is attributed to the presence of its d-orbitals. Previous research has documented both theoretical and experimental studies pertaining to these specific halides [38-40].

CONCLUSION

The objective of this study is to investigate the structural, and electronic properties of Magnesium-based halides using the FP-LAPW technique. The findings on all parameters of Mg based halides indicate that these materials have the potential to be synthesised under normal atmospheric conditions. These include the lattice parameter, the bulk modulus, the first derivative of the bulk modulus, the minimum energy, and the volume. The structural properties match up with the experimental data. Electronic properties in terms of the band structure (BS) and total and partial density of state (T-DOS and P-DOS) profiles of CsMgCl$_3$ using GGA potentials exhibit an indirect wide energy band gap of 5.35 eV. All these properties show that the CsMgCl$_3$ compound is used as a perovskite in solar cells.

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ДОСЛІДЖЕННЯ СТРУКТУРНИХ ТА ЕЛЕКТРОНИХ ВЛАСТИВОСТЕЙ СПОЛУКИ CsMgCl₃

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У цій роботі ми досліджували сполуку CsMgCl₃ за допомогою програмного пакету WIEN2K. Структурні та електронні властивості визначалися з використанням методу повнопотенційних приєднаних плоских хвиль (FP-LAPW) з наближенням узагальненого градієнта (GGA) як обмінних кореляційних потенціалів. Ми використовували рівняння Берча-Мурнагана (BME) визначення структурних властивостей матеріалу. До них відносяться параметр решітки, модуль об'ємного стиску, перша похідна модуля об'ємного стиску, мінімальна енергія та об'єм. Структурні властивості відповідають експериментальним даним. Електронні властивості з точки зору зонної структури (BS), а також профілів повної та парціальної густини станів (T-DOS та P-DOS) CsMgCl₃ з використанням потенціалів GGA демонструють непряму широку енергетичну заборонену зону 5,35 eB. Всі ці властивості показують, що з'єднання CsMgCl₃ може бути використаний як перовскітна структура в сонячних елементах.

Ключові слова: *GGA; оптоелектроніка; генератор енергії; заборонена зона*