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First-Principles Calculation on Structural, Electrical and Optical Properties of APbI3 (A=CH3NH3, Cs) for Perovskites Solar Cell Applications by using Spin-Orbit-Coupling (SOC)

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ABSTRACT

Methylammonium Lead Iodide ($CH_3NH_3PbI_3$) and Cesium Lead Iodide ($CsPbI_3$) are two of the most promising materials for perovskite solar cells (PSCs) applications because of their remarkable optimal bandgap, high absorption coefficient and broad absorption spectrum. Both materials are positioned as an active absorber layer. The structural, electronic and optical properties of PSCs are still difficult to precisely determine in their understanding and optimization. In this work by using density functional theory (DFT), structural, electronic and optical properties have been investigated and conducted by first-principles calculations using the Cambridge Serial Total Energy Package (CASTEP) within Generalized Gradient Approximation (GGA) parameterized by Perdew-Burke-Ernzerhod (PBE) calculations. First principle study has been compared in this research with the previous theoretical and experimental result. Due to variations in fabrication techniques, film quality, and experimental methods and also different type of computer codes with different bandgap that has been reported bandgap (~1.48–1.70 eV) varies slightly for CH3NH3PbI3 and CsPbI3. The (Spin-Orbit Coupling) SOC effect has to be incorporated as it majorly lessens the bandgap by causing an evident splitting of the first degenerated conduction levels. By using SOC the best band gap has been found which is 1.34 eV and 0.97 eV for CsPbI3 and CH3NH3PbI3, respectively. With the help of the dielectric function, the optical properties were thoroughly examined through optical simulations the organic-inorganic perovskite CH3NH3PbI3 and CsPbI3 characteristic is verified. According to experimental results, the estimated static refraction index value is 2.47. This approach not only aims to resolve discrepancies in the reported data but also establishes a comprehensive understanding of these materials, advancing their potential in optoelectronic applications.

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1. Introduction

Renewable energy has gained popularity in the late 20th century due to the depletion of fossil fuels and their environmental impact[1]. In terms of consumer demand, solar energy is currently one of the most popular renewable energy sources. Solar cells also known as photovoltaic (PV) cells, are regarded as one of the most important environmentally friendly power sources. They use the PV effect to transform light energy into electricity [2]. Four major generations can be used to broadly classify the evolution of different PV technologies over time. The most widely used solar cells on the market are first-generation (1G) solar cells, which come in single and multi-crystalline silicon varieties. Despite having high power conversion efficiencies (PCEs), first-generation solar cells are also expensive to produce. To further lower the cost, second-generation (2G) solar cells based on copper indium gallium selenide (CIGS), amorphous silicon, and cadmium telluride were created. Third-generation (3G) emerging solar cell technologies were developed as a result of the fact that 2G solar cells frequently perform worse than 1G solar cells. Third-generation (3G) emerging solar cell technologies have gained popularity recently in the research community due to the abundance of opportunities for exploration[3]. While, the Fourth-generation (4G) has not been discover yet. Fig. 1 shows that example of three major generations.

Among these 3G solar cell technologies, PSCs are the one that is developing the fastest and can produce electricity effectively at a low cost. Recently, PSC has been considered as possible Power Conversion Efficiency (PCE) material because of their remarkable optical and electronic characteristics including their long charge carrier diffusion length, narrow band gap, high absorption coefficient [4]. Even though silicon-based photovoltaics currently hold a dominant market share with an efficiency of up to 23%, perovskites-based PVs show the fastest rate of improvement in solar cells power conversion efficiency (PCE), rising to 25.2% in just ten years [5]. In recent years, $CH3NH3PbI_3$and $CsPbI_3$ one of the most promising materials in PSC that is called hybrid halide perovskite, has been extensively researched for use as an absorbance layer in solar cells[6]. Additionally, following the discovery and synthesis of a novel material composition known as perovskites, which have the general structure ABX_3 and are described as three-dimensional lattices with octahedral locations in their corners , extensive research is being done to learn more about this class of materials. Because of their great efficiency, affordability and adaptability perovskite solar cell (PSCs) are a new kind of solar technology that is gaining popularity [7]. In 1970s, PSC are a new class of materials that were created by scientists who modified A-components with various organic substitutes. The chemical structure, phase transitions, and absorption characteristics of PSC have been hot topics in the scientific community both initially and for a long time after they were materialised[8]. The typical formula for PSC materials with ABX_3 structure whereas group A is organic-inorganic metal (Cs and CH3NH3), at the center is metal cations B (Pb) and Halogen anion X (I-). Methylammonium Lead Iodide ($CH_3NH_3PbI_3$) and Cesium Lead Iodide ($CsPbI_3$) has been investigated in this research due to their exceptional optimal bandgap, high absorption coefficient, and broad absorption spectrum. However, there is a significant gap in research on $CsPbI_3$ and phase of information among other perovskite and have been gradually emphasized.

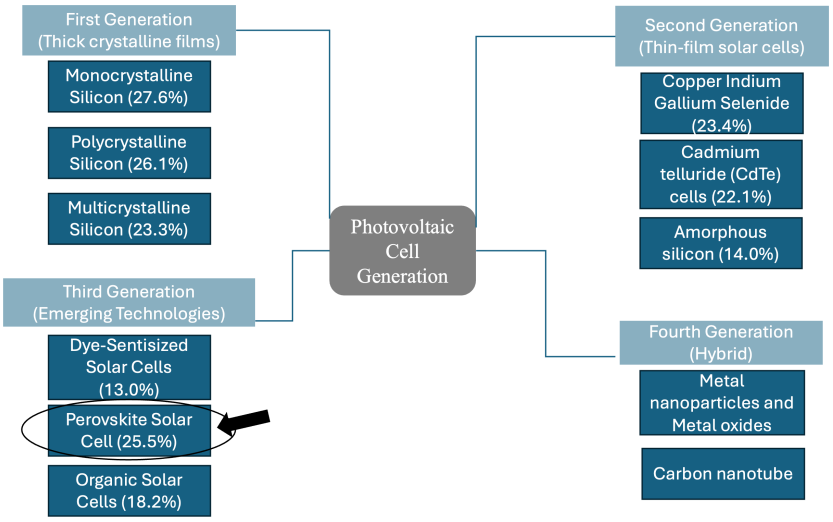

Fig. 1. Example of Generation solar cells and also the highest PCE for every materials

DFT based on the GGA-PBE scheme is the most widely used theoretical approach in the extensive theoretical investigation of both CsPbI3 and CH3NH3PbI3. By using local exchange correlational functionals, it is able to obtain bandgaps that are consistent with the experimental ones while saving computational costs [9]. In DFT , spin–orbit coupling (SOC) has a significant impact on the bandgap reduction calculations, causing a significant splitting of the first degenerate conduction level and a significant underestimation of the bandgap[10]. Nevertheless, this concurrence without SOC is coincidental and results from significant error cancellations. According to some researchers, the Rashba band splitting brought on by the SOC should be taken into account in order to obtain a low recombination rate for solar cells. Regarding the SOC in a material's electronic band structure, there are two main factors. First, while maintaining spin degeneracy, spin–orbit coupling causes the orbitals within the band to split [11].In this work has been report, a comprehensive and systematic DFT study of two halide perovskites by using density functional theory calculations on electronic and optical properties lead-based perovskite APbI3 (A=CH3NH3, Cs) using first principle approach.

2. Methodology

2.1 Structural Modelling

The process of building models of structures or systems to study their behaviour , stability and response to different circumstances is known as structural modelling By using the Cambridge Serial Total Energy Package (CASTEP) module of Material Studio, we performed First Principle DFT calculations with a plane wave basis for this study [12]. By using Vanderbilt-type ultrasoft pseudopotentials, the valance electron-ion core electrostatic interaction was estimated. With very little accuracy loss, the ultrasoft pseudopotentials reduce computation time [10-14]. Using the Perdw-Burke-Ernzerhof (PBE) and PBEsol exchange correlation functional, a Generalised Gradient Approximation (GGA) was utilized to analyze the electronic exchange and the correlation energy with and without spin orbit coupling (SOC) [15]. It becomes essential to include the SOC effect when heavy atoms such as lead(Pb) are present. We have considered a 550 eV cutoff energy for the Monkhorst-Pack scheme methylammonium for ensuing simulation of the consequent Brillouin zone. All structures were modelled using the unit cells of the cubic phase with space group Pm-3m (#221), as illustrated in Fig 2. CsPbI3 and CH3NH3PbI3 perovskites were sampled using a 9 x 6 x 9 K-point sampling grid [16].

2.2 Optimization of Properties

Structural properties (lattice parameter, volumes, bond length and structural stability),Electronic properties (band structure, partial and total density of state, atomic population from Mulliken population analysis and electron density), Optical properties (dielectric function, refractive index, loss function, reflectivity and absorption coefficient) has been analyzed [17].

3. Results And Discussion

3.1 Structural Properties

An unit cell that consists of 12 atoms, with 8-atom organic cation $CH_3NH_3^+$ or Cs^+ the cubic perovskite structure ABX^3 ($A=CH_3NH_3$, Cs , B=Pb , X=I) has been investigated. Here is the atomic composition of the elements: A: 1 s 2 2 s 2 2p6 3 s 2 3p6 3d10 4 s 2 4p6 5 s 1 , Pb: 1s2 2s2 2p6 3s2 3p6 3d104s2 4p6 4d104f145s2 5p6 5d106s1 and I: 1s2 2s2 2p6 3s2 3p5 [18] . According to previous research, cubic phase has high stability and efficient than other phases that can often associated with optical performance for light absorption. It is associated with space group Pm-3m, number 221. A single unit cell is shown in Figure 1a and Figure 1b with an 8-atom organic cation occupying the body-centered position at the 1b Wyckoff position with fractional coordinates (1/2,1/2,1/2). The single unit cell has 12 atoms total. In the Wyckoff position, the metallic cation Pb^{2+} is located at Figure 1 fractional coordinates of (0,0,0) while the I^- anion occupies 3d fractional coordinates of (1/2,0,0) [19]. The results for lattice parameter have been compared result with experimental data collected at 100K as shown in Table 2, the calculated structural parameters are acceptable. As previously stated, the DFT method was used to calculate the ground state at 0 K. As a result, the variation between our findings and the experimental data match expectations are tabulated including lattice and volume. Furthermore, the cubic crystal's lattice properties very slightly change at low temperatures, which helped to explain why the percentage difference is tiny. Additionally, the result has been compared with other different computer codes and other experimental values.

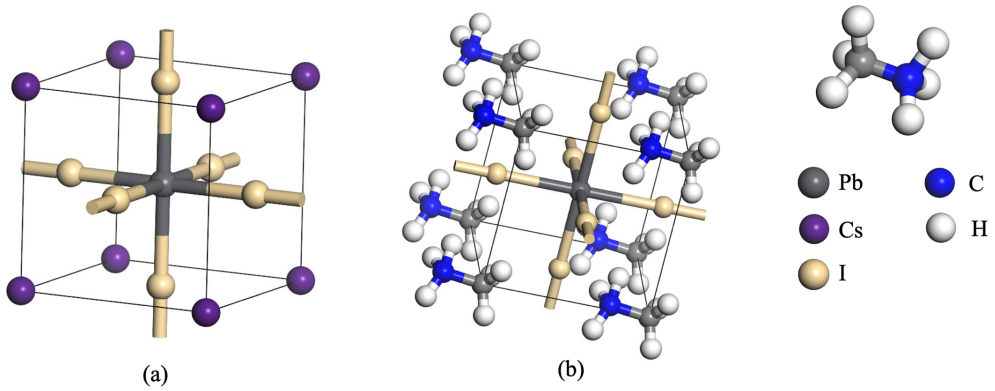

Fig. 2. Schematic view of unit cell of (a)CsPbI3 and (b)CH3NH3PbI3

Table 1
Structural parameter on cubic phase for CH3NH3PbI3 and CsPbI3 with standard GGA-PBEsol

Material	Functional	Lattice Parameter (Å)			Volume(Å^3)
		a	b	c	
CH3NH3PbI3	GGA-PBE	6.28 (0.78%)	6.28 (0.78%)	6.28 (0.78%)	247.67 (2.35%)

Table 1 (*Continued*)

	Calculated GGA-PBE	6.34	6.37	6.35	[5]
	Exp.	6.33	6.33	6.33	253.63[20]
CsPbI3	GGA-PBE	5.79 (8.90%)	5.79 (9.24%)	5.79 (9.24%)	194.10 (24.19)
	Calculated GGA-PBE	5.73	5.7	5.7	[21]
	Exp.	6.29	6.38	6.38	256.03[22]

3.2 Electronic Properties

Electronic properties characteristics play a key role to determine its capacity in harvest light. Such as finding lowest bandgap and contribution of various orbital of different atoms in density of states (DOS) are the main factor for the best material in perovskite [23]. Table 3 list the calculated band gap obtained using the DFT method, without using SOC and with SOC. Figure 2 which is devoted to the semiconductor material, illustrates the variation of band structure by using different functional. The band structures of the cubic CsPbI3 crystal has been presented and calculated along the high-symmetry lines in the first Brillouin zone. Upon closer inspection, it is evident that both display a direct band gap at the R symmetry with calculated band gaps of 2.31 eV and 0.97 eV without SOC and with SOC respectively which the valance band maximum (VBM) and conduction band minimum (CBM) crossed at an equivalent k-point of Brillouin zone has showed. On the other hand, the result for CH3NH3PbI3 is entirely coincidental because error cancellation occurs in an ultrasoft pseudopotential with partial DOS. The accuracy of band gap calculations can be improved with the use of hybrid functional on DFT methods. GW method and by evaluating the SOC but due to computational limitations the proper treatment on band gap calculations remains difficult on our side. Not with standing, the technical aspect the result obtained demonstrate a strong correlation with earlier research demonstrating that inorganic metal cations have a significant impact on hybrid halide.

Table 2
Band gap data with and without SOC calculated with standard GGA-PBE

Material	Band Gap (Eg)	
	Without SOC	With SOC
CH3NH3PbI3	2.73	1.93
CsPbI3	2.31	0.97

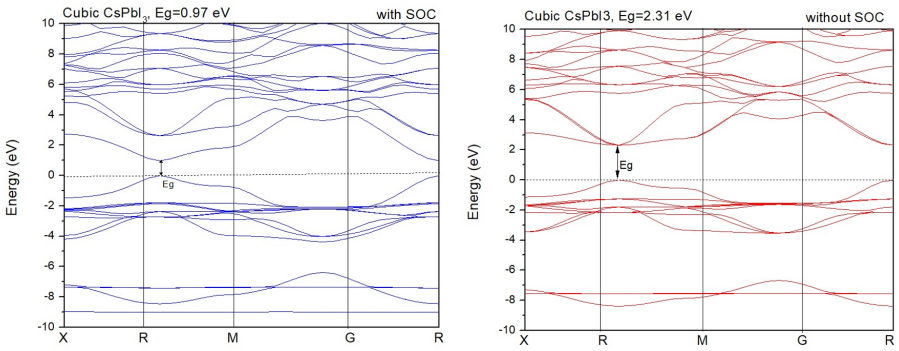

Fig. 3. Band structure of cubic CsPbI3

3.3 Optical Properties

Optical characteristics are important because they represent how electromagnetic waves interact with matter [24]. Thus, they are an important indicator in choosing a material for optical application. In this research, all six functionals have been calculated the dielectric constant, refractive index, absorption spectrum, conductivity, reflectivity and energy loss function for a denser k-mesh of (4x4x4) at a cut off energy of 550 eV in order to fully comprehend the optical response of cubic CsPbI3 [25].

The formula for the dielectric function is,

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega) \quad (1)$$

Where $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ represent the real and imaginary components of the dielectric function respectively [26]. The imaginary part clarifies the absorption, and real part explains the refractive index [27].

$$\varepsilon_1(\omega) = 1 + \frac{2}{\pi}\int_0^\infty \frac{\varepsilon_2(\omega')\omega'}{\omega'^2-\omega^2}\, d\omega' \quad (2)$$

$$\varepsilon_2(\omega) = \frac{2e^2\pi}{\Omega e_0}\sum_{k,v,c}|\langle\psi_k^c|\hat{u}r|\psi_k^v\rangle|^2\,\delta(E_k^c - E_k^v - E) \quad (3)$$

The linear response of the system to electromagnetic radiation can be expressed in terms of the dielectric function $k(\omega)$, Its imaginary part, n(ω) which is associated with the materials electronic absorption can be computed from the electronic structure using DOS and the matrix elements that separate the occupied and unoccupied wave functions inside the selection criteria [15]. The Krames-Kronig transformation can be used to derive the real part $k(\omega)$ of the dieletric function from the imaginary part as shown in Fig. 3 [28]. The relation of extinction coefficient $k(\omega)$ and absorption coefficient $\alpha(\omega)$, with the dielectric function can be defined by the following mathematical formula:

$$k(\omega) = \left(\frac{|\varepsilon(\omega)|-\varepsilon_1(\omega)}{2}\right)^{1/2} \quad (4)$$

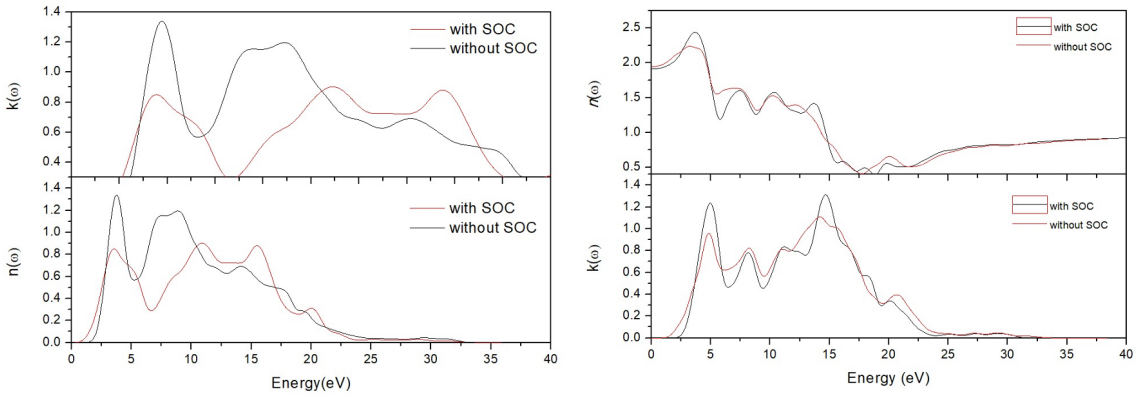

Fig. 4. Refractive index of (a)CsPbI3 and (b)CH3NH3PbI3

The maximum peak of CH3NH3PbI3 is shown in Figure 4 with a value of 1.32 at 7.8 eV and 2.67 at 4.89 eV with SOC. Whereas without SOC have the lowest value of the index of refraction(n) 0.82 at 4.7eV and 2.15 at 4.76 eV. Since all of the light will be absorbed, there won't be any transmittance at high energies (lower wavelengths) Transmission will be very strong in this range, though, because there are no pertinent electronic transitions at low energies (longer wavelengths) [29].

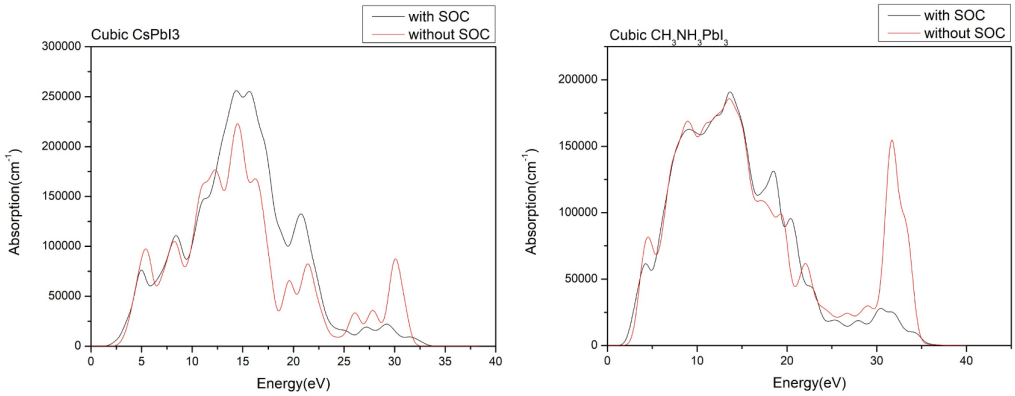

Fig. 5. Absorption coefficient of (a) $CsPbI_3$ and (b) $CH_3NH_3PbI_3$

The absorbance of the substances is computed using the standard relationship:

$$I(\omega) = 2^{1/2}\omega[\{\varepsilon_1{}^2(\omega) + \varepsilon_1{}^2(\omega)\}^{1/2} - \varepsilon_1(\omega)]^{1/2} \quad (5)$$

In Figure 5 shows that the comparison for both result of absorption coefficient of CsPbI3 and CH3NH3PbI3 with and without SOC. As shown in the figure CsPbI3 with SOC has the maximum absorption peak, with a peak value of 27344.29 at 14.90 eV whereas without SOC the peak decrease to 23544.42 at 13.76eV and the lowest value for the absorption peak value is 1934221.42 at 15.67 eV with SOC and decrease to 172342.65 at 14.78 eV for CH3NH3PbI3. According to this study, by comparing these types of materials, it show that the compounds of concern with the highest UV absorption values have a high concentration of free carriers [30].

4. Conclusions

In conclusion, we have studied the accuracy of the calculation by performing a theoretical calculation on the structural, electronic, and optical properties of cubic phase for ABX_3 (A=CH_3NH_3, Cs; B=Pb; X=I) using various approximations. By examining the band structure, the effects of incorporating spin-orbit coupling (SOC) in computation are examined. Surprisingly, a narrower band gap is the better result obtained by combining the GGA function with SOC. The results of the optical absorption analysis using SOC with two different materials indicate negligible differences. Otherwise, $CsPbI_3$ and CH3NH3PbI3 is a perfect absorber material for solar cells due to its high absorption of light in both UV and visible regions.

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