

# Electronic Structure and Optical Response of $\text{Cs}_2\text{AgSbBr}_6$ : A Lead-Free Double Perovskite for Sustainable Photovoltaics

Fahd Elmourabit<sup>1\*</sup>, Yassine Essakali<sup>1</sup>, Fatima Id Ouissaaden<sup>1</sup>, Hamza Kamel<sup>1</sup>, Mohssin Aoutoul<sup>1</sup>, and Said Dlimi<sup>1</sup>

<sup>1</sup>Laboratory of Sciences and Technologies of Information and Communication (LSTIC), Team: Microelectronic, Microwaves, Instrumentation and Information (MM2I), Physics Department, Faculty of Sciences, Chouaib Doukkali University, El Jadida 24000, Morocco

**Abstract.** In photovoltaics applications, lead-free double-halide perovskites are attracting increasing attention as a sustainable replacement for lead-based perovskites. This article investigates the behaviour of photons and electrons by using a computer code called CASTEP. The calculation results show an indirect band gap of 1.361 eV, which places this substance in an energy range suitable for solar-energy conversion. The energy band structure shows that the carrier mobility is asymmetric, meaning that electrons are lighter and holes are heavier. A detailed examination of the band edge energy levels reveals that the valence band is controlled by a mixture of Ag-Br hybridization, and the conduction band is controlled by a combination of Sb-p hybridisation. There were no deficiencies in the middle band. The absorption of visible light begins at the band gap, is followed by moderate absorption, and then low reflectivity with a relatively high static refractive index. These results suggest that  $\text{Cs}_2\text{AgSbBr}_6$  is a promising lead-free optoelectronic and photovoltaic material.

## 1 Introduction

The rapid evolution of photovoltaic technologies has positioned halide perovskite materials at the forefront of next-generation solar energy research, making them a key component in the development of advanced solar cells and other related technologies. Lead-based perovskites have exhibited remarkable optoelectronic characteristics, allowing certified power conversion efficiencies of over 25% and tending to the theoretical boundaries of single-junction devices (National Renewable Energy Laboratory [NREL], 2025). Although these lead-based perovskites have awesome optoelectronic performance, their practical use is still limited by toxicity concerns and instability in the long run. This has led to a lot of effort to find eco-friendly alternatives that have similar electronic and optical properties. Consequently, considerable research endeavours have been focused on lead-free perovskite-inspired compounds, with halide double perovskites exhibiting the general composition  $\text{A}_2\text{B}^+\text{B}^{3+}\text{X}_6$  proving to be a particularly promising class. Through the substitution of  $\text{Pb}^{2+}$  with pairs of monovalent and trivalent cations, such as ( $\text{Ag}^+$ ,  $\text{Bi}^{3+}$ ) or ( $\text{Ag}^+$ ,  $\text{Sb}^{3+}$ ), these materials ensure charge neutrality while markedly diminishing ecological and health hazards. So, there's been a lot of research recently that shows how double perovskites are better than lead-based ones in terms of how strong they are, how well they resist moisture and how stable they are at high temperatures [1]. This has

made them more popular for use in solar panels and other electronic devices.

Out of all the systems,  $\text{Cs}_2\text{AgBiBr}_6$  has been the one that's been looked at the most, because it's stable and can tolerate defects well. Experiments and computer simulations have shown that it lasts a long time and is not easily damaged. Nevertheless, its comparatively broad and indirect bandgap (~2.0eV) considerably reduces visible-light absorption, thus constraining achievable photovoltaic efficiencies [2]. The motivation for exploration of alternative cationic configurations capable of improving optical activity without compromising stability has been this intrinsic limitation. A strategy that shows great promise involves substituting  $\text{Bi}^{3+}$  with  $\text{Sb}^{3+}$ , which results in the emergence of  $\text{Cs}_2\text{AgSbBr}_6$  as a viable lead-free absorber candidate. When  $\text{Sb}^{3+}$  is introduced, it changes the way the electrons are arranged in the atoms and makes the band edges line up. This creates a bandgap that is located within the visible spectral range and causes a moderate increase in optical absorption. Lately, scientists have been studying how well these materials work and how they can be used to make solar panels. They have found that these materials are good at capturing light and can be changed to suit different uses [3-5].

The basis of the  $\text{Cs}_2\text{AgSbBr}_6$  study was a broader framework of numerical and design-oriented modelling methods. The effectiveness of these methods in improving photovoltaic efficiency in various material systems has been demonstrated. In this regard, recent studies by Elmourabit et al. have revealed how advanced

\* Corresponding author: [elmourabit.fahd@ucd.ac.ma](mailto:elmourabit.fahd@ucd.ac.ma)

numerical modelling can be used to investigate the role of absorber thickness. They also look at charge carrier concentration. In addition, they consider the engineering of the bandgap. Mechanisms of recombination in CdS/CdTe thin-film solar cell systems are another area of interest [6]. The same applies to triple-cation perovskite halide devices. High tolerance to variation in parameters was reported for the work's device architectures, and in the case of triple-cation perovskites, efficiencies greater than 34% were simulated, while unresolved issues related to lead-based toxicity and durability were also highlighted [7]. The transition from lead-based absorbers toward lead-free double perovskites such as  $\text{Cs}_2\text{AgSbBr}_6$  can therefore be viewed as a logical continuation of these earlier investigations, extending established modeling methodologies to a new class of sustainable materials. Lessons derived from chalcogenide heterostructures and multi-cation perovskites particularly regarding defect tolerance, carrier transport optimization, and bandgap tailoring provide a solid foundation for assessing the photovoltaic viability of Sb-based double perovskites. In view of the given context, the aim of the present work is the provision of a comprehensive examination of the electronic and optical properties of  $\text{Cs}_2\text{AgSbBr}_6$ , with specific reference to its suitability as a lead-free (PV) photovoltaic solar absorber. The combination of knowledge from recent literature and advanced computational and theoretical perspectives is the object of this work, with the meaning of clarifying the strong points of the material, identifying its current limitations and contributing to the broader effort promoting sustainable and eco-friendly photovoltaic energy technologies.

## 2 METHOD AND MATERIALS

First-principles calculations using the CASTEP code of the Materials Studio software package have been used to study the structural, electronic and optical characteristics of lead-free double perovskite  $\text{Cs}_2\text{AgSbBr}_6$ . Researchers have widely used this computational approach to study the energy stability, electronic structure and optical response of halogenated perovskites and lead-free material-inspired perovskites, especially for photovoltaic and optoelectronic applications [8, 10].

### 2.1 Structural Optimization

All calculations were executed using the generalized gradient approximation (GGA) in conjunction with the PBEsol exchange-correlation functional, as evidenced by its superior performance in determining the lattice parameters and equilibrium volumes of crystalline solids [9, 15]. The description of the electron-ion interaction was with ultra-soft pseudo-potentials, allowing for efficient plane-wave representation with high computational accuracy. The convergence of the total energy and stress tensor was ensured by using a 570-eV plane wave kinetic cut-off, in line with the convergence requirements for metal-halide perovskites and related compounds [10]. The Brillouin zone integration was carried out using a  $6 \times 6$

$\times 6$  Monkhorst-Pack k-point grid, resulting in sufficient reciprocal space sampling for the cubic crystal structure of  $\text{Cs}_2\text{AgSbBr}_6$  [13, 14].

We achieved complete relaxation of the crystal structure through simultaneous optimization of the lattice parameters and atomic internal coordinates. Convergence thresholds were established at  $10^{-6}$  eV per atom for total energy and  $0.01\text{eV}/\text{\AA}$  for maximum residual force, thereby ensuring a robust approximation of the ground-state geometry [3, 14].

### 2.2 Electronic Structure

Structural relaxation was followed by electronic band structure and density of states (DOS) calculations to investigate the nature of the band gap and orbital contributions around the Fermi level. The experimental results evaluated the bandgap dispersion across the high symmetry points of the Brillouin zone, specifically  $\Gamma$ , X, L, and W As shown in Fig. 1 and the Fig.2. This allows for the accurate identification of the valence band maximum ( $V_{\text{BM}}$ ) and the conduction band minimum ( $C_{\text{BM}}$ ), as it also determines whether the semiconductor has a direct or indirectly forbidden bandgap. This is an important criterion for performance in photovoltaics [4, 5]. The GGA-based functionals are known to be slightly too weak when it comes to measuring the energy gap between the bands, however they are still useful in showing where the bands are shifting and which ones are most important for transporting electricity and reflecting or absorbing light [1, 8].

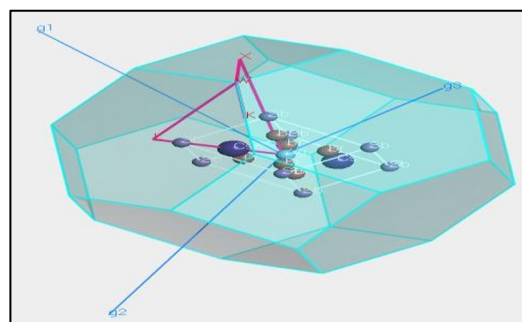


Fig 1. First Brillouin Zone

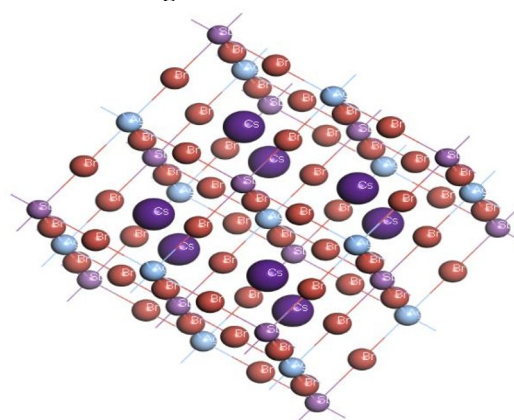


Fig 2. High-Symmetry Path for the Double Perovskite  $\text{Cs}_2\text{AgSbBr}_6$

It should be noted that the band gap value obtained within the GGA-PBEsol model should be slightly underestimated, as is commonly reported for semi-local

exchange-correlation functionals. This limitation stems from the intrinsic approximation of the exchange potential and the absence of discontinuity derived in conventional DFT formulations. Therefore, the calculated indirect band gap of 1.361 eV should be considered a minimum estimate of the true band gap of the quasiparticles.

Nevertheless, GGA-based calculations remain highly reliable for analyzing band dispersion, orbital contributions, and relative electronic trends. Since the main objective of this study is to elucidate the characteristics of the electronic structure and optical response mechanisms rather than to provide an absolute experimental prediction of the band gap, the methodology adopted remains entirely appropriate. More advanced approaches, such as hybrid functionals or many-body perturbation methods, could refine the quantitative value, but should not alter the qualitative conclusions drawn in this work.

### 2.3 Optical Properties

The nature of the interaction between light and  $\text{Cs}_2\text{AgSbBr}_6$  was determined using a formula (1) involving complex dielectric functions, obtained using a method called independent particle approximation.

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

The comprehensive dielectric function explains the optical characteristics of our double perovskite, including  $\varepsilon_1(\omega)$  the real part, which is related to light dispersion and polarization effects, and the Imaginary part  $\varepsilon_2(\omega)$ , directly linked to the transitions between various electron energy state levels and optical absorption. Important optical properties were extracted from this dielectric function, including the absorption coefficient ( $\alpha$ ), the reflectivity (R), the refractive index (n), as well as the extinction coefficient (k).

From the relation (1), the refractive index  $n(\omega)$  and the extinction coefficient  $k(\omega)$  are gotten as:

$$n(\omega) = \sqrt{\frac{|\varepsilon(\omega)| + \varepsilon_1(\omega)}{2}} \quad (2)$$

$$k(\omega) = \sqrt{\frac{|\varepsilon(\omega)| - \varepsilon_1(\omega)}{2}} \quad (3)$$

where:

$$|\varepsilon(\omega)| = \sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)} \quad (4)$$

These have been extracted over a photon energy range of 0 to 35 eV, spanning the visible and ultraviolet spectral ranges [10].

The interaction between light and matter and the suitability of  $\text{Cs}_2\text{AgSbBr}_6$  as a photovoltaic solar absorber are evaluated based on these optical properties. The material's ability to collect solar radiation is represented by the absorption coefficient ( $\alpha$ ). The index of refraction (n) and extinction coefficient explain how light travels and weakens inside the crystal  $k(\omega)$ .

$$\alpha(\omega) = \frac{2\omega k(\omega)}{c} \quad (5)$$

where:

- $c$  : is the speed of light in vacuum,
- $\lambda$  : is the wavelength of the incident light.

The normal-incidence reflectivity is given by:

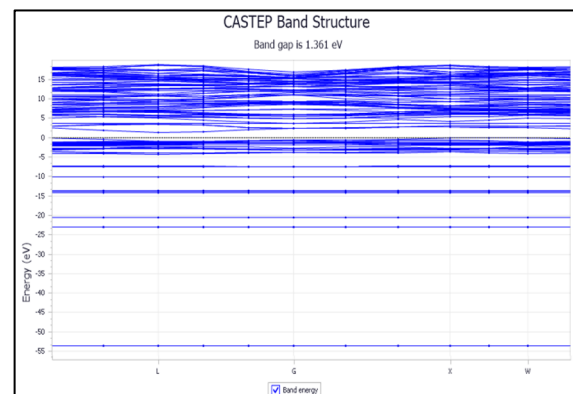
$$R(\omega) = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2} \quad (6)$$

## 3 Results and Discussion:

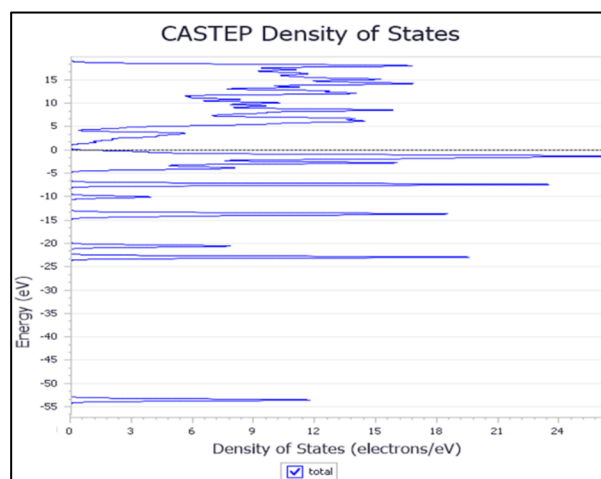
### 3.1 Electronic Band Structure and Density of States

We calculated the band structure of  $\text{Cs}_2\text{AgSbBr}_6$  (Fig. 3), clearly revealing an indirect band gap of 1.361 eV. We found that the valence band maximum ( $V_{BM}$ ) and the conduction band minimum ( $C_{BM}$ ) are located at distinct high-symmetry k-points located along the  $L-\Gamma-X-W$  path. This observation clearly indicates the presence of an indirect band gap, a feature well known for double halide perovskites due to the rules that govern the mixing of elements and the bonding of atoms [2, 4, 5]. The energy gap value we obtained in this work is practically the same as that reported by other works based on first principles, which usually report indirect energy gaps of around 1.3 to 1.6 eV for  $\text{Cs}_2\text{AgSbBr}_6$ , based on the exchange-correlation functional used [3, 5]. Importantly the value achieved for the band gap lies within the optimal energy window expected by the Shockley-Queisser detailed limit for single-junction photovoltaic devices, which increases the potential suitability of  $\text{Cs}_2\text{AgSbBr}_6$  as an absorbing material [11]. Therefore, it appears that  $\text{Cs}_2\text{AgSbBr}_6$  is a very promising absorber material, at any rate from an energy perspective.

A more detailed inspection of the energy band dispersion reveals that the conduction bands are comparatively dispersive, implying low effective electron masses and advantageous electron transport properties. In comparison, the energy valence bands show a flatter dispersion, implying heavier effective hole masses and a potentially lower hole mobility. This mismatch between electron and hole carrier transport has been consistently found in double perovskites with antimony and bismuth and is a key reason for the limited charge extraction performance in photovoltaic systems [1, 8].



(a)



(b)

**Fig. 3.** (a) Electronic Band Structure and (b) DOS of  $\text{Cs}_2\text{AgSbBr}_6$ 

However, such an imbalance in transport doesn't prevent photovoltaic performance, providing that appropriate transport layers or interface design strategies are employed.

The density of states (DOS) calculation further clarifies the electronic origin of the structure of the observed band. As shown in Figure 3 (b), the edge of the valence band is composed mainly of Ag-4d states and Br-4p states, whereas the edge of the conduction band is composed mainly of Sb-5p orbitals. This orbital configuration is fully compatible with previously published theoretical reports on  $\text{Cs}_2\text{AgSbBr}_6$  and related compounds [3, 5]. It will be noted that no intermediate states are observed, indicating the lack of defect-induced electronic states in the band gap, which confirms the high intrinsic electronic quality of the material and affirms its tolerance to defects, a crucial advantage for photovoltaic stability [10].

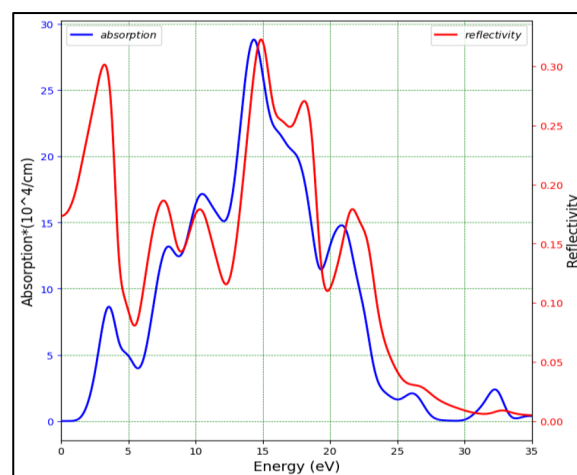
Comparing  $\text{Cs}_2\text{AgBiBr}_6$ , which has already been extensively researched and has a significantly larger indirect band gap (~1.9-2.0eV), we can see that replacing  $\text{Bi}^{3+}$  with  $\text{Sb}^{3+}$  in  $\text{Cs}_2\text{AgSbBr}_6$  results in a substantial reduction in the band gap. This is due to the different energy locations and hybridization forces of the Sb-5p and Bi-6p states, resulting in improved absorption of visible light, as highlighted in numerous scientific studies [2-4]. Although the indirect nature of the bands gap remains a major limitation near the absorption edge, the advantage of Sb substitution clearly improves the photovoltaic potential of the compound [12].

### 3.2 Optical Absorption and Reflectivity

The blue curve in Figure 4 represents the calculated absorption spectrum of  $\text{Cs}_2\text{AgSbBr}_6$ . This spectrum shows the presence of absorption in the 1.3–1.5 eV range, which is very similar to the indirect band gap that was determined from the structural electronic configuration. This observation confirms the semiconductor character of the compound and is in

perfect accordance with previous optical studies using DFT [3, 10].

In the optical spectrum, the quantity of light absorbed is not excessively high, which indicates that the major change is not directly related. This constraint is frequently observed in double halide perovskites and is the main obstacle to achieving high photovoltaic conversion efficiency in this class of materials [4]. Nevertheless, the absorption is significantly increased compared to  $\text{Cs}_2\text{AgBiBr}_6$ , which has a large band gap that strongly limits visible light capture. At elevated photon energies, the pronounced absorption peaks are observed in the UV region (5–20eV), with values exceeding  $2.5 \times 10^5 \text{ cm}^{-1}$ . This intensity is attributable to interband excitations involving the Br-4p, Ag-4d, and Sb-5p states, as demonstrated by DOS analysis. Earlier theoretical investigations have reported a similar high-energy absorption behaviour, which is characteristic of metal-halide structures with strong p-d hybridisation [3, 10].

**Fig 4.** Optical Absorption and Reflectivity of Lead-Free Double Perovskite  $\text{Cs}_2\text{AgSbBr}_6$ 

The reflectivity spectral curve (Fig. 4, red curve) appears relatively low across the entire energy range studied, typically below 0.3. The points where light is most reflected coincide with those where light absorption is significant, indicating substantial variations in electron energy levels across the band. The combination of low reflectivity and absorption over a broad spectrum in the UV region makes  $\text{Cs}_2\text{AgSbBr}_6$  particularly attractive for use in optoelectronic and environmental-friendly UV photo-detector applications, as well as for photovoltaics. However, further optimisation, such as band engineering, stress modulation or heterostructure design, is necessary to increase the absorption in the visible range and fully exploit its photovoltaic potential.

In general, the present results using DFT-CASTEP demonstrate remarkable concordance with previous theory and experiments, both in the band gap magnitude and the orbitals character of the band gaps. The computations used in this work are robust, as is demonstrated by the agreement with several other independent reports. The validity of the conclusions in this study is therefore confirmed. Moreover, the

narrower band gap obtained here, when compared to some previous results, provides further evidence of the potential of double-based antimonium perovskites. They may represent an improved replacement for bismuth-based perovskites. This is important for sustainable photovoltaic technologies.

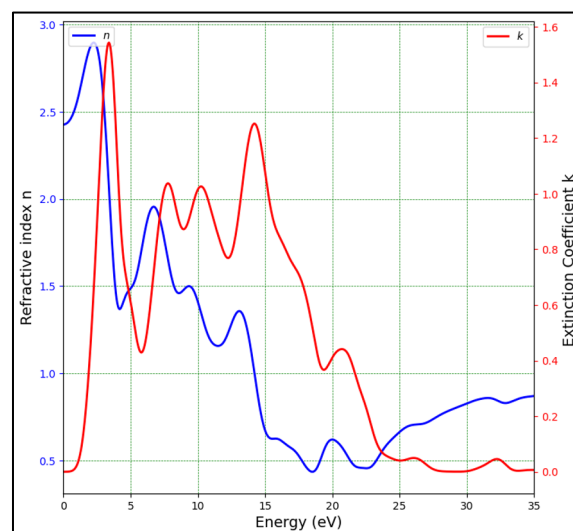
### 3.3 Optical Dispersion: Refractive Index and Extinction Coefficient

As illustrated in Figure 5, the dispersion behavior of  $\text{Cs}_2\text{AgSbBr}_6$  can be defined by the variation of refractive index ( $n$ ) and the extinction coefficient ( $k$ ) across a wider range of photon energies. The optoelectronic response of the material can be interpreted by analyzing these two parameters, which give complementary details about the absorption and propagation mechanisms of optical waves.

The index of refraction is relatively high at low photonic energies, with a static value of  $n_{(0)} \approx 2.5\text{--}2.9$ . These values are like those reported for other halogenated perovskites and lead-free double perovskites [2, 10]. Such high refractive indexes indicate high light-matter interaction and good photonic confinement. These properties are desirable for photovoltaic absorbers and photonic components, as they enhance the internal trapping of light and increase the optical path length.

The  $n$  and  $k$  maxima are approximately 2eV, which corresponds closely to the absorption edge of  $\text{Cs}_2\text{AgSbBr}_6$ . This is closely related to the onset of interband transitions across the indirect band gap, as has been determined previously from the electronic band gap structure. The simultaneously increasing  $n$  and  $k$  near the band edge suggests a strong coupling relationship between the electronic transitions and the optical dispersions, a widely documented phenomenon in indirect bandgap semiconductor materials [3, 4].

There is a clear observation of a change in the spectrum between the  $n$  and  $k$  peaks. This feature highlights the interplay between absorption and dispersion, which are intricately governed by Kramers-Kronig relations. Under these relations, variations in the extinction coefficient related to electronic transitions result in reciprocal adjustments in the index of refraction. The researchers discovered that  $\text{Cs}_2\text{AgSbBr}_6$  and related double perovskites exhibit similar behaviour in light scattering. This is consistent with the fact that their optical response is dominated by transitions that involve the Br-4p, Ag-4d, and Sb-5p orbitals. This is also supported by the analysis of the density of states [5, 10]. The material is almost transparent once the main interband transitions are exhausted, as the extinction coefficient drops rapidly to very low values at higher photon energies, notably those above approximately 20 electron volts. In this high-energy regime, a more uniform variation in the refractive index is also observed, approaching a weakly dispersive behaviour. This observation is consistent with previous theoretical research on lead-free double-halide perovskites and confirm that the pronounced optical activity of  $\text{Cs}_2\text{AgSbBr}_6$  is limited mainly to the Visible and Near-Ultraviolet (NUV) spectra [3].



**Fig 5.** Optical Dispersion of  $\text{Cs}_2\text{AgSbBr}_6$ : Refractive Index and Extinction Coefficient

In comparison to  $\text{Cs}_2\text{AgBiBr}_6$ , which has been widely studied, and which generally exhibits smaller refractive indices in the visible range due to its larger band gap ( $\sim 2.0\text{eV}$ ), the antimonium-based compound shows improved spectral dispersion near the band edge, which confirms the advantageous role of antimonium substitution in improving light-matter interactivity. However, the indirect bandgap nature still limits the absorption efficiency at low photon energies, implying that additional techniques such as bandgap engineering, strain tuning, or hetero-structure design are required to fully exploit its photovoltaic performance.

Overall, the index of refraction and Extinction Coefficient spectrums provide robust and independent confirmation of the electronic band structure analysis and optical absorption results discussed previously. The combined effect of a high static refractive index strongly defined dispersion characteristics near the band edge, and decreased absorption losses at higher energy levels highlights  $\text{Cs}_2\text{AgSbBr}_6$  as a promising lead-free material for optoelectronic and PV applications, while also clarifying the intrinsic limitations imposed by its indirect band gap.

## 4 General Discussion and Implications

In general, the electrical and optical results obtained in this work are in perfect agreement with previous experimental and theoretical studies, thus verifying the DFT-CASTEP methodology employed. The antimony-based  $\text{Cs}_2\text{AgSbBr}_6$  perovskite clearly exhibits better visible light absorption and higher optical dispersion than its Bismuth-based counterpart, while also maintaining high structural robustness and defect tolerance. While the indirect bandgap continues to be a limiting factor for overall photovoltaic efficiency, the advantageous bandgap value, low-reflectivity, and strong light-matter interaction are compelling attributes for  $\text{Cs}_2\text{AgSbBr}_6$  as a lead-free candidate for sustainable photovoltaic and optoelectronic device technologies.

## 5 Conclusion

This work offers a detailed, fundamental-principles-based evaluation of the lead-free double perovskite  $\text{Cs}_2\text{AgSbBr}_6$ , focussing on the intrinsic links between its structural and optical properties. The computed indirect bandgap of 1.361eV places this compound in a substantial energy range for photovoltaic device applications, meanwhile the band dispersion indicates a clear distinction between electron and hole transport, which is typical of halide double perovskites. An examination of the band edge shows that the valence band consists of Ag-Br blends, and the conduction band consists of Sb-p states. there are no signs of undesirable intermediate states.

Optical calculations show moderate visible-light absorption, high ultraviolet interband transitions, and a comparatively high static refractive index, which suggests an efficient interaction between matter and light. A smaller band gap and improved optical performance are the result of replacing Sb with Bi-based analogues. While the indirect band gap remains a limiting factor, these results demonstrate that  $\text{Cs}_2\text{AgSbBr}_6$  provides a solid foundation for further engineering of the band structure and interface for sustainable photovoltaic technologies.

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