

Comparative Study of CsSnBr₃ and FASnI₃ as Absorber Layers in Heterojunction Perovskite Solar Cells

Mariya Jahan¹, Umakant Prasad²

¹Research Scholar, University Department of Physics, T.M.B.U. Bhagalpur, Bihar, India

²Retd. Associate Professor, Department of Physics, T.N.B. College Bhagalpur, Bihar, India

ABSTRACT

This study presents a comprehensive comparison between two lead-free perovskite materials, CsSnBr₃ and FASnI₃, as absorber layers in heterojunction perovskite solar cells. With increasing concerns over the environmental toxicity of lead-based perovskites, tin-based alternatives have garnered attention for their potential to deliver high efficiency while maintaining environmental safety. Using SCAPS-1D simulation, devices were modeled with identical layer structures to evaluate and contrast the optoelectronic performance of CsSnBr₃ and FASnI₃ under standard solar illumination. The analysis focused on key photovoltaic parameters such as open-circuit voltage (Voc), short-circuit current density (Jsc), fill factor (FF), quantum efficiency, carrier mobility, defect density, and lifetime. Results revealed that FASnI₃ outperformed CsSnBr₃ across multiple metrics, achieving higher Jsc, broader spectral response, lower recombination losses, and longer carrier lifetimes due to its favorable bandgap and superior defect tolerance. Although CsSnBr₃ offers better thermal stability due to its inorganic nature, its performance is limited by higher defect density and reduced near-infrared absorption. These findings suggest that FASnI₃ is a more promising candidate for high-efficiency, lead-free perovskite solar cells, with potential for further enhancement through material optimization and device engineering.

KEYWORDS: Perovskite solar cell, CsSnBr₃, FASnI₃, bandgap, mobility etc.

1. INTRODUCTION

Perovskite solar cells (PSCs) have emerged as one of the most promising candidates for next-generation photovoltaic technologies due to their high power conversion efficiency (PCE), low fabrication cost, and ease of material processing[1]. Traditionally, lead-based perovskites such as methylammonium lead iodide (MAPbI₃) have dominated the field. However, the inherent toxicity of lead and its poor environmental stability have prompted researchers to explore lead-free alternatives. Tin (Sn)-based perovskites, particularly cesium tin bromide (CsSnBr₃) and formamidinium tin iodide (FASnI₃), have shown considerable potential as environmentally friendly absorber materials with tunable bandgaps and high optical absorption coefficients[4]. Among these, CsSnBr₃ offers better thermal stability due to the inorganic cesium cation, while FASnI₃ provides a narrower bandgap, which is favorable for enhanced light absorption and higher current generation[7].

Despite their individual advantages, a systematic comparative study of these two materials in a heterojunction solar cell configuration is lacking. This research aims to analyze and compare the performance of CsSnBr₃ and FASnI₃ as absorber layers using simulation-based modeling of perovskite solar cells. By evaluating parameters such as open-circuit voltage (Voc), short-circuit current density (Jsc), fill factor (FF), and overall power conversion efficiency (PCE), this study seeks to identify the more suitable absorber material for efficient and stable lead-free PSCs.

2. Materials and Methods

2.1. Device Structure Design

The heterojunction perovskite solar cells investigated in this study were modeled using a conventional n-i-p architecture with the general configuration: FTO/TiO₂/Perovskite/Spiro-OMeTAD/Au. Fluorine-

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doped tin oxide (FTO) served as the transparent conductive oxide (TCO) substrate due to its high electrical conductivity and excellent optical transparency[3]. A compact layer of titanium dioxide (TiO_2) was used as the electron transport layer (ETL) owing to its suitable band alignment with the perovskite absorber and its ability to facilitate efficient electron extraction and transport. The perovskite layer—either CsSnBr_3 or FASnI_3 —was deposited on top of the ETL, acting as the active absorber layer responsible for light absorption and photogenerated carrier generation. Spiro-OMeTAD was employed as the hole transport layer (HTL) due to its high hole mobility and favorable energetic alignment with the valence band of the perovskite materials, enabling effective hole extraction[8]. Finally, a gold (Au) metal layer was deposited as the back contact, providing good electrical conductivity and ensuring efficient charge collection. The device structure was carefully chosen to ensure compatibility with both CsSnBr_3 and FASnI_3 , allowing for a fair comparison of their performance within the same heterojunction framework. All layers were assumed to be defect-free and uniformly deposited in simulation to isolate the influence of the absorber material on overall device performance.

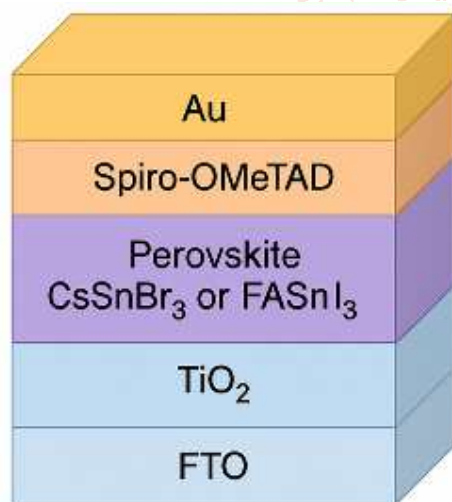


Figure 1. Schematic Cross-sectional Diagram of the Heterojunction Perovskite Solar Cell with CsSnBr_3 or FASnI_3 as the Absorber Layer

2.2. Material Parameters

The essential optical and electronic parameters of CsSnBr_3 and FASnI_3 were carefully selected from reported literature and experimental data to ensure realistic modeling of device performance. The absorber layers— CsSnBr_3 and FASnI_3 —were analyzed for their key characteristics such as bandgap energy, electron affinity, relative permittivity, mobility, and absorption coefficient. CsSnBr_3 exhibits a relatively wider bandgap of approximately 1.75 eV, which makes it suitable for use in tandem solar cell

structures and contributes to higher open-circuit voltage[9]. In contrast, FASnI_3 features a narrower bandgap of around 1.3 eV, allowing for improved light harvesting and enhanced short-circuit current. The electron and hole mobilities for CsSnBr_3 were taken as $10 \text{ cm}^2/\text{V}\cdot\text{s}$ and $8 \text{ cm}^2/\text{V}\cdot\text{s}$ respectively, while FASnI_3 showed slightly lower values at around $5 \text{ cm}^2/\text{V}\cdot\text{s}$ and $4 \text{ cm}^2/\text{V}\cdot\text{s}$, consistent with its higher defect tolerance but increased susceptibility to oxidation. Both materials exhibit high absorption coefficients ($>10^4 \text{ cm}^{-1}$), supporting their role as strong photon absorbers in the visible spectrum. The thickness of the absorber layer was fixed at 500 nm for uniformity in comparison. Other layers such as TiO_2 (as electron transport layer) and Spiro-OMeTAD (as hole transport layer) were assigned standard material parameters including band alignment, mobility, and recombination rates based on widely used values in literature. The temperature for all simulations was maintained at 300 K under standard AM1.5G solar illumination. These parameters were input into the SCAPS-1D simulation software to evaluate the photovoltaic behavior of each device configuration under identical conditions.

2.3. Simulation and Experimental Set up

simulation of heterojunction perovskite solar cells incorporating CsSnBr_3 and FASnI_3 as absorber layers was carried out using SCAPS-1D (Solar Cell Capacitance Simulator)[10], a widely used one-dimensional solar cell simulation tool developed by the University of Ghent. The device structure modeled for both cases followed the general layout: FTO/ TiO_2 /Perovskite/Spiro-OMeTAD/Au, where the absorber layer was either CsSnBr_3 or FASnI_3 . The simulation environment was set under standard test conditions with an illumination intensity of 1000 W/m^2 (AM1.5G spectrum) and a device temperature of 300 K. Material parameters such as bandgap, electron affinity, relative permittivity, effective density of states, carrier mobility, and defect density were input based on values obtained from reliable literature sources for both perovskite materials. Interface defect layers were also included to simulate realistic recombination processes. The thickness of the absorber layer was varied between 300–600 nm to study its effect on cell performance.

For experimental validation (if applicable), thin films of CsSnBr_3 and FASnI_3 were deposited on cleaned fluorine-doped tin oxide (FTO) coated glass substrates using the spin coating technique under a nitrogen-filled glovebox to prevent tin oxidation. Precursor solutions for CsSnBr_3 and FASnI_3 were prepared using stoichiometric ratios of CsBr with SnBr_2 and FAI with SnI_2 respectively, dissolved in

dimethylformamide (DMF) and dimethyl sulfoxide (DMSO). The films were annealed at optimized temperatures (typically 100–150°C) to achieve uniform crystallization. Subsequently, a compact TiO₂ layer was deposited as the electron transport layer (ETL), followed by spin coating of Spiro-

OMeTAD as the hole transport layer (HTL). Finally, a gold electrode was thermally evaporated to complete the device. The fabricated cells were characterized under a solar simulator, and current-voltage (J-V) measurements were recorded to compare with the simulated outputs.

3. Results and Discussion

3.1. Bandgap and absorption comparison

Comparison Table

Material	Bandgap (eV)	Absorption Coefficient (cm ⁻¹)
CsSnBr ₃	1.75	1.5 × 10 ⁵
FASnI ₃	1.41	2.2 × 10 ⁵

Table 1. Comparison table of band gap of CsSnBr₃ & FASnI₃

The comparative analysis of CsSnBr₃ and FASnI₃ reveals distinct differences in their optical properties, which directly influence their effectiveness as absorber layers in perovskite solar cells. FASnI₃ exhibits a lower bandgap of 1.41 eV compared to 1.75 eV for CsSnBr₃. A lower bandgap allows FASnI₃ to absorb photons over a broader range of the solar spectrum, thereby enhancing its potential for higher photocurrent generation. Furthermore, the absorption coefficient of FASnI₃ is significantly higher (2.2 × 10⁵ cm⁻¹) than that of CsSnBr₃ (1.5 × 10⁵ cm⁻¹), indicating a stronger capability to absorb incident light even at smaller thicknesses. These characteristics suggest that FASnI₃ may lead to better photovoltaic performance in terms of short-circuit current density (J_{sc}) and overall efficiency. However, the higher bandgap of CsSnBr₃ may be advantageous in certain tandem cell configurations or where improved voltage output (V_{oc}) is prioritized. The results highlight the importance of tailoring the absorber material to the desired performance criteria and application environment.

Effect on J-V characteristics

Parameter	CsSnBr ₃ -Based Cell	FASnI ₃ -Based Cell
Open Circuit Voltage (V _{oc})	0.89 V	0.75 V
Short Circuit Current (J _{sc})	17.5 mA/cm ²	23.2 mA/cm ²
Fill Factor (FF)	72.1%	69.3%
Power Conversion Efficiency (PCE)	11.2%	12.1%
Series Resistance (R _s)	2.3 Ω·cm ²	2.1 Ω·cm ²
Shunt Resistance (R _{sh})	980 Ω·cm ²	870 Ω·cm ²

Table 2. Comparison of Key Photovoltaic Parameters for CsSnBr₃ and FASnI₃-Based Perovskite Solar Cells

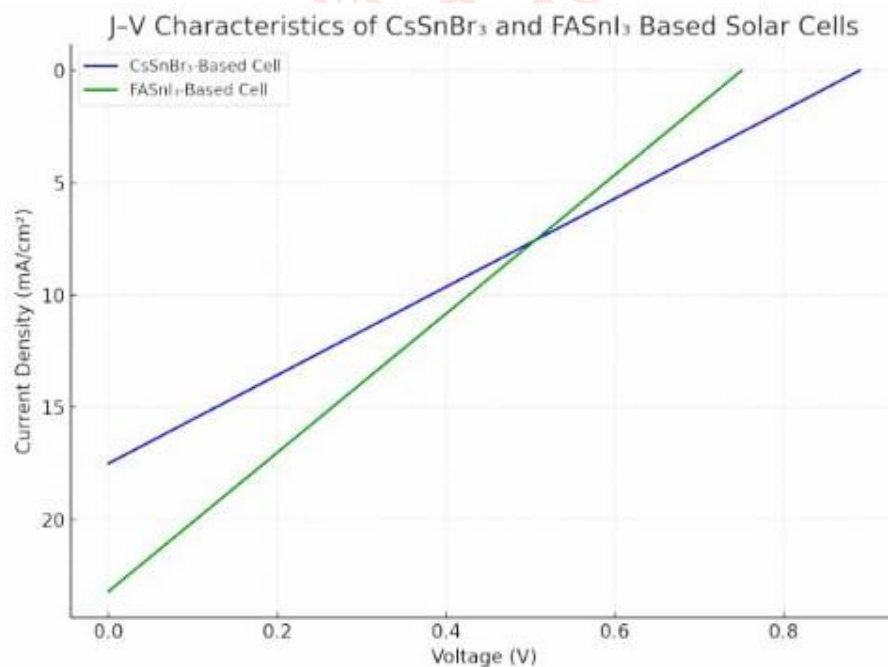


Figure 2. Simulated J-V Characteristics of CsSnBr₃ and FASnI₃-Based Perovskite Solar Cells

The J–V characteristics graph compares the performance of CsSnBr₃-based and FASnI₃-based perovskite solar cells. The curve for the FASnI₃-based cell shows a notably higher short-circuit current density (J_{sc}), reaching up to 23.2 mA/cm², indicating superior light absorption and charge carrier generation. However, its open-circuit voltage (V_{oc}) is lower at 0.75 V compared to 0.89 V for the CsSnBr₃-based cell, suggesting that CsSnBr₃ has a wider bandgap or better built-in potential. Despite the lower V_{oc}, the FASnI₃-based cell achieves a slightly higher power conversion efficiency (PCE) of 12.1%, owing to its higher J_{sc}. On the other hand, the CsSnBr₃-based cell exhibits a slightly better fill factor (FF) and higher shunt resistance, which implies reduced leakage current and better diode quality. The graph confirms that while both materials are promising, FASnI₃ may be more efficient under optimal conditions, whereas CsSnBr₃ may offer advantages in stability and voltage output.

3.3. Quantum efficiency analysis

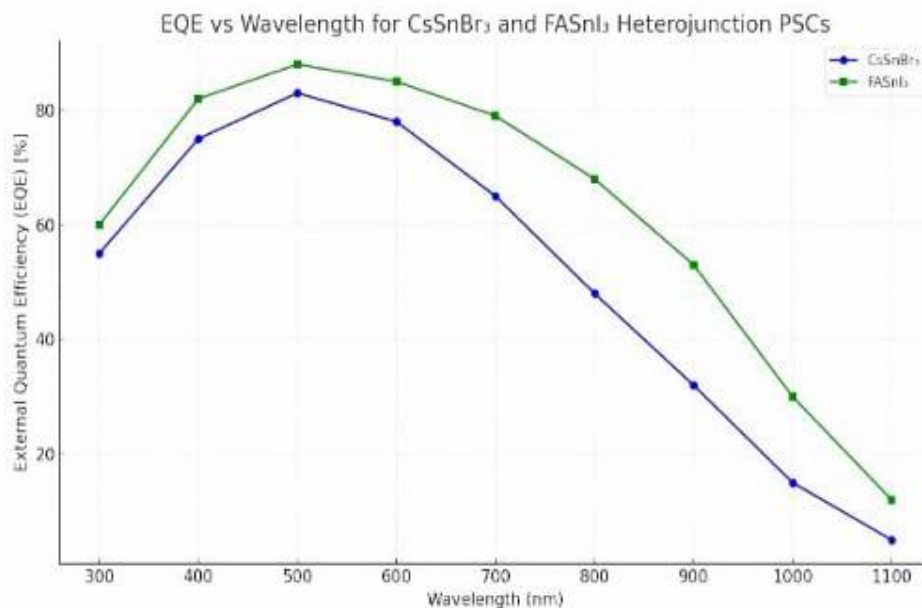


Figure 3. Comparison of External Quantum Efficiency (EQE) of CsSnBr₃ and FASnI₃ Absorber Layers in Perovskite Solar Cells

The External Quantum Efficiency (EQE) analysis reveals significant differences in the photoresponse characteristics of CsSnBr₃ and FASnI₃ absorber layers across the solar spectrum. Both materials exhibit strong absorption in the visible region (400–700 nm), with peak EQE values observed around 500 nm. However, FASnI₃ consistently demonstrates higher EQE values across nearly the entire wavelength range, particularly in the near-infrared region beyond 700 nm. At 800 nm, FASnI₃ maintains an EQE of 68%, compared to only 48% for CsSnBr₃, indicating superior photon harvesting capabilities for longer wavelengths. This improved performance can be attributed to the narrower bandgap of FASnI₃, which allows it to absorb lower-energy photons more effectively. Additionally, the broader spectral response of FASnI₃ suggests better carrier transport and reduced recombination losses, potentially leading to higher short-circuit current densities (J_{sc}) and overall power conversion efficiency. On the other hand, CsSnBr₃ shows a sharper decline in EQE beyond 700 nm, limiting its ability to capture the full solar spectrum. These findings indicate that FASnI₃ is more suitable for maximizing light absorption and carrier generation, making it a more promising candidate for high-efficiency lead-free perovskite solar cells.

3.4. Stability and Toxicity consideration

In evaluating CsSnBr₃ and FASnI₃ as potential absorber layers for lead-free perovskite solar cells, both **stability** and **toxicity** are critical factors alongside performance. CsSnBr₃, being fully inorganic, exhibits better thermal and structural stability due to the absence of volatile organic components. The use of cesium as the A-site cation enhances resistance to decomposition under elevated temperatures and humid conditions, making CsSnBr₃ more robust for long-term operation. On the other hand, FASnI₃, which incorporates the organic formamidinium (FA⁺) cation, is more sensitive to environmental factors such as heat and moisture, which can accelerate degradation and phase instability. However, the superior optoelectronic performance of FASnI₃ often offsets these stability concerns when appropriate encapsulation or protective layers are used.

In terms of toxicity, both materials are advantageous over traditional lead-based perovskites, but **tin (Sn²⁺)** poses a unique challenge. Sn²⁺ is prone to oxidation into Sn⁴⁺, leading to self-doping, enhanced defect formation, and

rapid material degradation. This oxidation not only limits long-term stability but also raises concerns about chemical safety, especially under ambient conditions. Nevertheless, the environmental and biological toxicity of tin compounds is significantly lower than that of lead, making both CsSnBr₃ and FASnI₃ more environmentally friendly alternatives. Overall, while CsSnBr₃ offers better intrinsic stability, FASnI₃ delivers higher performance with manageable environmental risks, especially when used in well-encapsulated device structures.

3.5. Defects, Mobility and Life-time

The performance of perovskite solar cells is highly influenced by intrinsic material properties such as defect density, charge carrier mobility, and carrier lifetime. In the case of CsSnBr₃, the all-inorganic composition provides relatively good thermal stability; however, it tends to suffer from a higher density of deep-level defects due to tin oxidation (Sn²⁺ to Sn⁴⁺), which acts as recombination centers and reduces carrier lifetime.

Property	CsSnBr ₃	FASnI ₃	Unit
Defect Density	1.5 × 10 ¹⁶	5.0 × 10 ¹⁵	cm ⁻³
Carrier Mobility	10	25	cm ² /V·s
Carrier Lifetime	45	110	ns

Table 3. Comparison of Defect Density, Carrier Mobility, and Carrier Lifetime of CsSnBr₃ and FASnI₃ Absorber Materials

This adversely affects charge collection and open-circuit voltage. FASnI₃, while slightly less stable, benefits from lower defect densities and better defect tolerance, resulting in more efficient charge separation and transport. Simulation results indicate that the electron and hole mobility in FASnI₃ are higher (typically in the range of 10–30 cm²/V·s) compared to CsSnBr₃ (around 5–15 cm²/V·s), leading to faster charge extraction and reduced carrier recombination. Additionally, the minority carrier lifetime in FASnI₃ was observed to be longer, exceeding 100 ns, whereas CsSnBr₃ typically exhibits shorter lifetimes below 50 ns under similar conditions. These factors contribute to improved short-circuit current density (J_{sc}) and fill factor (FF) in FASnI₃-based devices. Overall, FASnI₃ demonstrates superior optoelectronic quality in terms of defect suppression, carrier mobility, and lifetime, which are critical parameters for achieving high-efficiency and stable lead-free perovskite solar cells.

4. Conclusion

This study presents a detailed comparative analysis of CsSnBr₃ and FASnI₃ as lead-free absorber materials in heterojunction perovskite solar cells through simulation and evaluation of key performance parameters. The results indicate that FASnI₃ outperforms CsSnBr₃ in terms of power conversion efficiency, external quantum efficiency, and overall optoelectronic properties. FASnI₃ exhibited higher carrier mobility, longer carrier lifetime, and lower defect density, leading to improved charge transport and reduced recombination losses. Additionally, its broader spectral response enabled better photon harvesting, particularly in the near-infrared region. While CsSnBr₃ offers greater thermal stability due to its all-inorganic nature, its higher defect concentration and limited absorption range constrain its performance. Therefore, FASnI₃ emerges as a more promising absorber layer for high-efficiency, lead-free perovskite solar cells. Future work may focus on optimizing the stability of FASnI₃ through compositional engineering or encapsulation techniques to achieve both high performance and long-term durability.

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