



RESEARCH ARTICLE

Optimizing the Performance of Lead-free $\text{CH}_3\text{NH}_3\text{SnI}_3$ Perovskite Solar Cells via Thickness, Doping, and Defect Density Control

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HIGHLIGHTS

- $\text{CH}_3\text{NH}_3\text{SnI}_3$ perovskite is a promising alternative for efficient and environmentally friendly solar cells.
- The researchers achieved a high-power conversion efficiency of 23.9% in the optimized cell.
- The use of lead-free perovskite materials can reduce manufacturing costs and improve environmental sustainability.

Keywords:

- Perovskite solar cells,
- Photovoltaic performance,
- Manufacturing process,
- Lead-free perovskite,
- Numerical simulation.

GRAPHICAL ABSTRACT

This study focuses on $\text{CH}_3\text{NH}_3\text{SnI}_3$ perovskite as a lead-free alternative for solar cells. The researchers used one-dimensional simulation software to investigate the photovoltaic properties of $\text{CH}_3\text{NH}_3\text{SnI}_3$ perovskite solar cells with a $\text{TiO}_2/\text{CH}_3\text{NH}_3\text{SnI}_3/\text{Cu}_2\text{O}$ structure. The thickness of the absorbing layer, doping concentration, and density of defects were adjusted to improve the performance of the solar cells. The obtained results demonstrate that $\text{CH}_3\text{NH}_3\text{SnI}_3$ perovskite has the potential to be an efficient and environmentally friendly absorber. The researchers achieved a high-power conversion efficiency (PCE) of 23.9%, along with a high short-circuit current density (J_{sc}) of 31,519 mA/cm^2 , an open-circuit voltage (V_{oc}) of 0.965V, and a high fill factor (FF) of 78.7%. These results are encouraging and demonstrate the potential of $\text{CH}_3\text{NH}_3\text{SnI}_3$ perovskite as a promising alternative to $\text{CH}_3\text{NH}_3\text{PbI}_3$ for use in solar cells. Furthermore, the use of lead-free perovskite materials in solar cells could offer several advantages, including improved environmental sustainability and reduced manufacturing costs. It also opens opportunities for the development of more stable and efficient solar cells that can be produced on a large scale. However, more research is needed to further optimize the performance and stability of lead-free perovskite solar cells before they can be commercially viable.

Table A The name figure or table about given info and result

	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	PCE (%)
Reference cell	0,748	30,982	77,819	18,035
Optimized cell	0,965	31,519	78,717	23,943

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Aim of Article: The article aims to investigate and optimize $\text{CH}_3\text{NH}_3\text{SnI}_3$ perovskite as a lead-free alternative for solar cells to achieve higher efficiency and improved environmental sustainability.

Theory and Methodology: The theory and methodology of this work involve using $\text{CH}_3\text{NH}_3\text{SnI}_3$ perovskite as a lead-free alternative for solar cells, with the researchers utilizing one-dimensional simulation software to study its photovoltaic properties with a $\text{TiO}_2/\text{CH}_3\text{NH}_3\text{SnI}_3/\text{Cu}_2\text{O}$ structure. They adjusted the thickness of the absorbing layer, doping concentration, and density of defects to optimize the performance of the solar cells.

Findings and Results: The researchers found that $\text{CH}_3\text{NH}_3\text{SnI}_3$ perovskite can be a highly efficient and eco-friendly absorber for solar cells, achieving a high-power conversion efficiency (PCE) of 23.9% in the optimized cell. They also obtained a high short-circuit current density (J_{sc}) of 31,519 mA/cm^2 , an open-circuit voltage (V_{oc}) of 0.965V, and a high fill factor (FF) of 78.7%, demonstrating its potential as a viable alternative to $\text{CH}_3\text{NH}_3\text{PbI}_3$.

Conclusion : the use of $\text{CH}_3\text{NH}_3\text{SnI}_3$ perovskite as a lead-free alternative for solar cells shows promising results, with high power conversion efficiency and environmentally sustainable advantages. However, further research is needed to optimize the stability and performance of lead-free perovskite solar cells before they can be commercially viable.



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Optimizing the Performance of Lead-free $\text{CH}_3\text{NH}_3\text{SnI}_3$ Perovskite Solar Cells via Thickness, Doping, and Defect Density Control

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HIGHLIGHTS

- $\text{CH}_3\text{NH}_3\text{SnI}_3$ perovskite material as a promising lead-free alternative for perovskite solar cells.
- One-dimensional simulation software used to investigate the photovoltaic properties of $\text{CH}_3\text{NH}_3\text{SnI}_3$ perovskite solar cells with a $\text{TiO}_2/\text{CH}_3\text{NH}_3\text{SnI}_3/\text{Cu}_2\text{O}$ structure.
- Improved performance of $\text{CH}_3\text{NH}_3\text{SnI}_3$ perovskite solar cells achieved by adjusting the thickness of the absorbing layer, doping concentration, and density of defects.
- Obtained results demonstrate the potential of $\text{CH}_3\text{NH}_3\text{SnI}_3$ as a highly efficient and environmentally friendly solar absorber.
- The study highlights the importance of developing lead-free perovskite solar cells with high stability and efficiency for large-scale production.

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ABSTRACT

Perovskite solar cells have gained significant attention due to their excellent photovoltaic performance and simple manufacturing process. However, the use of lead (Pb) in the widely studied $\text{CH}_3\text{NH}_3\text{PbI}_3$ perovskite material limits its large-scale production due to low stability in the air. As a result, researchers have turned to lead-free $\text{CH}_3\text{NH}_3\text{SnI}_3$ perovskite as a promising alternative. In this study, we used one-dimensional simulation software to investigate the photovoltaic properties of $\text{CH}_3\text{NH}_3\text{SnI}_3$ perovskite solar cells with a $\text{TiO}_2/\text{CH}_3\text{NH}_3\text{SnI}_3/\text{Cu}_2\text{O}$ structure. By adjusting the thickness of the absorbing layer, doping concentration, and density of defects, we were able to improve the performance of the solar cells. The obtained results of $J_{sc} = 31,519 \text{ mA/cm}^2$, $V_{oc} = 0,965 \text{ V}$, $FF = 78,717\%$, and $PCE = 23,943\%$ demonstrate the potential of lead-free $\text{CH}_3\text{NH}_3\text{SnI}_3$ as a highly efficient and environmentally friendly solar absorber.

Keywords: Perovskite solar cells, Photovoltaic performance, Manufacturing process, Lead-free perovskite, Numerical simulation.

I. INTRODUCTION

Perovskite solar cells have garnered significant attention in recent years as a promising photovoltaic technology due

to their high efficiency and low-cost manufacturing process [1, 2]. In particular, the lead (Pb)-free hybrid perovskite $\text{CH}_3\text{NH}_3\text{SnI}_3$ has emerged as a strong contender for widespread use due to its high stability in the air and ability to achieve efficiencies over 25% [3, 4].



In this study, we used numerical simulation to investigate the photovoltaic properties of $\text{CH}_3\text{NH}_3\text{SnI}_3$ perovskite solar cells with a $\text{TiO}_2/\text{CH}_3\text{NH}_3\text{SnI}_3/\text{Cu}_2\text{O}$ structure. The obtained results demonstrate the potential of lead-free $\text{CH}_3\text{NH}_3\text{SnI}_3$ as a highly efficient and environmentally friendly solar absorber [13].

II. METHOD

Perovskite materials are a class of compounds with a specific crystal structure that have attracted a lot of interest in the field of solar cells because they have the potential to be more efficient and less expensive to produce than traditional solar cell materials. One perovskite that has been widely studied is $\text{CH}_3\text{NH}_3\text{SnI}_3$, which is a hybrid organic-inorganic material made up of tin, iodide, and methylammonium ions [12].

In a solar cell, the $\text{CH}_3\text{NH}_3\text{SnI}_3$ perovskite material is typically used as the light-absorbing layer, which converts sunlight into electrical energy. The efficiency of this conversion process can be improved by adding other layers or materials to the cell structure. For example, TiO_2 is often used as a scaffold material to help support the perovskite layer and improve its stability. Cu_2O is another material that has been explored for use in perovskite solar cells as a way to improve the device's ability to extract electrical charge carriers [14].

Overall, the use of perovskite materials and other layers or materials in solar cells is an active area of research and development, with the goal of developing more efficient and cost-effective solar energy technologies.

A. Reference Solar Cell Structure to Simulate

The purpose of the simulation of the reference solar cell structure is to study its performance and behavior under standard outdoor conditions, which include an illumination of 1000 w/m^2 at 300 K and an AM 1.5G air mass [11]. By simulating the solar cell structure, we can gain a better understanding of its underlying mechanisms and identify potential areas for improvement. The simulation allows for a detailed analysis of the electrical and optical properties of the solar cell, which can help in optimizing the design and improving the efficiency of the cell.

The reference solar cell structure is a planar structure consisting of three layers: TiO_2 , $\text{CH}_3\text{NH}_3\text{SnI}_3$, and Cu_2O , and is representative of a hybrid perovskite solar cell. The TiO_2 layer serves as an electron transport layer (ETL) and the front contact (anode) of the solar cell, while the $\text{CH}_3\text{NH}_3\text{SnI}_3$ layer is a p-type hybrid halide

perovskite material that functions as the light-absorbing layer [9]. The Cu_2O layer, on the other hand, is a p-type copper oxide material that serves as a hole transport layer (HTL) to the copper metal electrode (Figure1) [10].

By simulating this solar cell structure under standard conditions, we can gain insights into its performance and behavior, such as its current-voltage (IV) characteristics, power conversion efficiency (PCE), and spectral response. The simulation also allows for a comparison of the results with experimental data, which can provide validation for the simulation model. Ultimately, the goal of the simulation is to enhance the understanding of the solar cell structure's operation and to provide insights into potential improvements in its design and performance.

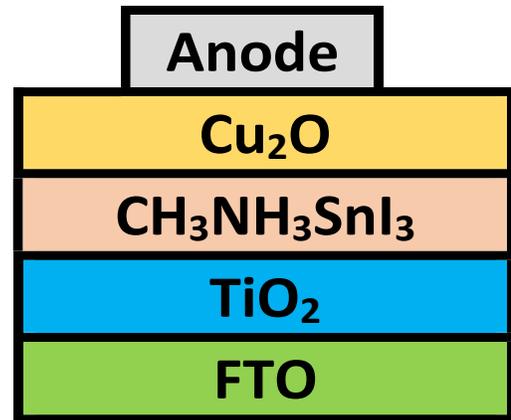


Figure. 1. Lead-free $\text{CH}_3\text{NH}_3\text{SnI}_3$ solar cell structure.

The energy levels of the studied solar cell are shown in Figure 2.

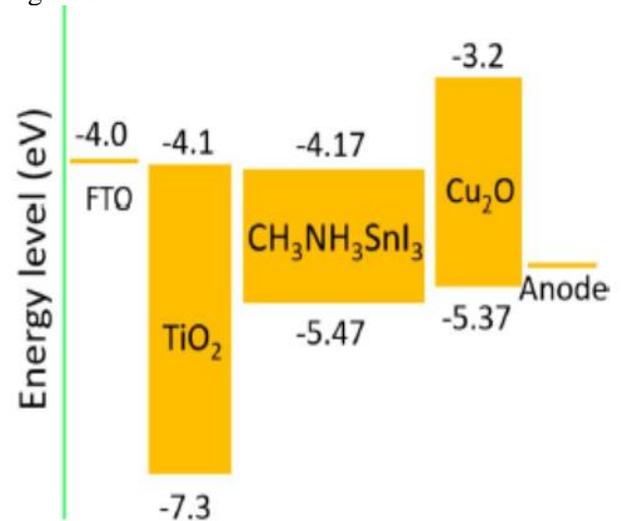


Figure. 2. Diagram of energy levels [5].



B. Reference Cell Parameters and Properties

The Reference Solar Cell (RSC) is a device used as a reference point for comparing the performance of different types of solar cells. It consists of three layers: a titanium dioxide (TiO₂) layer, a methylammonium tin iodide (CH₃NH₃SnI₃) layer, and a cuprous oxide (Cu₂O) layer. These layers have different thicknesses and properties that play a crucial role in determining the performance of the RSC. Table 1 summarizes the properties of these layers, including their thicknesses and electrical and optical properties. The TiO₂ layer is a wide bandgap n-type semiconductor that serves as the electron transport layer. The CH₃NH₃SnI₃ layer is a p-type semiconductor with a perovskite crystal structure that acts as the light-absorbing layer. The Cu₂O layer is a p-type semiconductor that acts as the hole transport layer. The properties of these materials, such as their bandgap energy, carrier mobility, and absorption coefficient, can be sourced from literature [5] and used to model the behavior of the RSC under various conditions.

To predict the performance of the RSC, it is important to consider the various operating conditions it may encounter. As mentioned earlier, these conditions include the intensity and spectrum of the incident light, temperature, humidity, and mechanical stress. By carefully specifying these conditions and incorporating them into the model, it is possible to accurately predict the performance of the RSC under a range of application conditions.

In addition to the properties of the individual layers, the cell also has interface parameters that describe the interactions between the layers. These parameters are listed in Table 2 [5] and may include information about the work function, the conduction and valence band offsets, and the surface recombination velocities at the interfaces. Understanding the interface parameters is important for predicting the overall performance of the cell and for optimizing its design.

The absorption coefficient of CH₃NH₃SnI₃ perovskite, shown in the figure below, was obtained from experimental data [6] and was imported into the software as a file. The absorption coefficient describes the ability of the material to absorb light and is an important parameter for predicting the performance of a solar cell. The figure 3 shows the absorption coefficient as a function of wavelength, which can be used to understand the material's spectral response and optimize its use in a solar cell. The data from reference [6] was used to input the absorption coefficient into the software, which can then be used to model the photovoltaic characteristics of the solar cell.

For the absorption coefficients of the Cu₂O and TiO₂ hole and electron transport layers (HTL and ETL), respectively, the SCAPS model was used. The absorption coefficients for these layers were calculated using the following equations:

Cu₂O HTL:

$$\alpha(\lambda) = A_1 \times \left(\frac{\lambda}{1000}\right)^{-B_1} \dots (1)$$

TiO₂ ETL:

$$\alpha(\lambda) = A_2 \times \left(\frac{\lambda}{1000}\right)^{-B_2} \dots (2)$$

In these equations, the absorption coefficient is a function of wavelength, which is divided by 1000 to convert it from nanometers to micrometers. The constants A₁, B₁, A₂, and B₂ are material-specific parameters that can be obtained from literature or experiments. Using these equations, the absorption coefficients of the Cu₂O and TiO₂ layers can be calculated for different wavelengths and used in the SCAPS model to predict the photovoltaic characteristics of the solar cell.

Table 1. Electrical and optical properties of the different layers of the cell

Parameters	FTO (TCO)	TiO ₂ (ETL)	CH ₃ NH ₃ SnI ₃	Cu ₂ O (HTL)
Thickness (nm)	500	120	450	100
Eg (eV)	3.4	3.2	1.3	2.17
χ (eV)	4.5	4.1	4.17	3.2
ε _r	9.1	9.0	8.2	7.1
N _c (cm ⁻³)	1.1*10 ¹⁹	2.2* 10 ¹⁸	1*10 ¹⁸	2*10 ¹⁷
N _v (cm ⁻³)	1.1*10 ¹⁹	1.8*10 ¹⁹	1*10 ¹⁸	1.1*10 ¹⁹
μ _n (cm ² /Vs)	20	0.05	2000	200
μ _p (cm ² /Vs)	10	0.05	300	80
ND (cm ⁻³)	1*10 ¹⁹	1*10 ¹⁸	0	0
NA (cm ⁻³)	0	0	1*10 ¹⁴	1*10 ¹⁸

Table 2. Parameters for the defects in materials and at interfaces.

Paramètres	TiO ₂	CH ₃ NH ₃ SnI ₃	Cu ₂ O	Interface TiO ₂ /CH ₃ NH ₃ SnI ₃	Interface CH ₃ NH ₃ SnI ₃ /Cu ₂ O
Defect type	Neutre	Neutre	Neutre	Neutre	Neutre
σ _n (cm ⁻²)	1*10 ⁻¹⁵	2.5*10 ⁻¹⁵	1* 10 ⁻¹⁵	1 * 10 ⁻¹⁵	1 * 10 ⁻¹⁵
σ _p (cm ⁻²)	1*10 ⁻¹⁵	8.5*10 ⁻¹⁵	1* 10 ⁻¹⁵	1 * 10 ⁻¹⁵	1 * 10 ⁻¹⁵
Energy distribution	Uniform	Gaussian	Uniform	Uniform	Uniform
Energy level with respect to E _v (above E _v) (eV)	0.600	0.650	0.100	0.600	0.600
Characteristic energy (eV)	-	0.100	-	-	-
N _t (cm ⁻³)	1* 10 ¹⁴	3.029*10 ¹⁶	1 * 10 ¹⁴	1 * 10 ¹⁰	1 * 10 ¹⁰

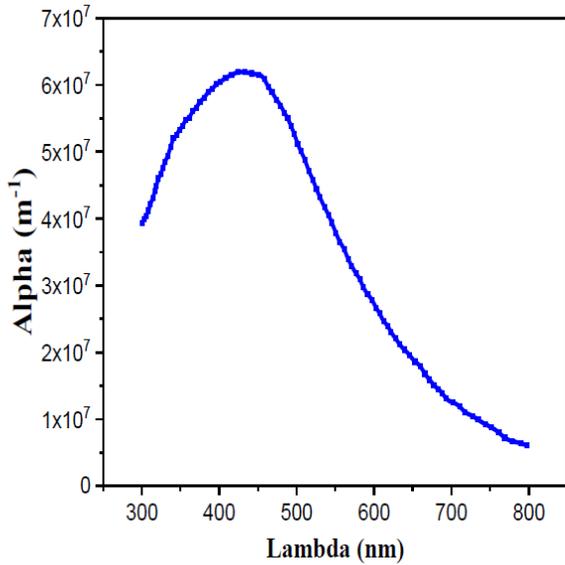


Figure 3. Absorption coefficient of CH₃NH₃SnI₃ perovskite

III. RESULTS AND DISCUSSION

A. Characteristic (J-V) and quantum efficiency QE

In introducing the parameters from Table 1 into the SCAPS simulator, we obtained the current density versus voltage (J-V) characteristic curve shown in Figure 4. From this curve, we were able to determine the photovoltaic parameters (J_{sc}, V_{oc}, FF, and η) for the cell under study. Figure 5 shows the external quantum efficiency of the cell as a function of wavelength (λ).

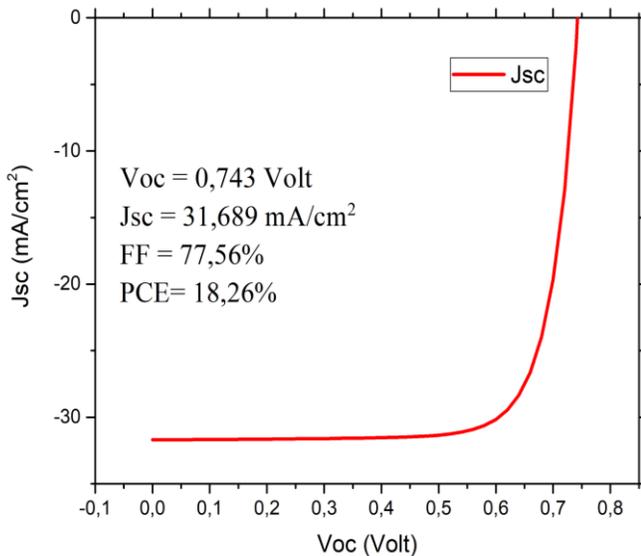


Figure 4. The current-voltage (J-V) characteristic curve.

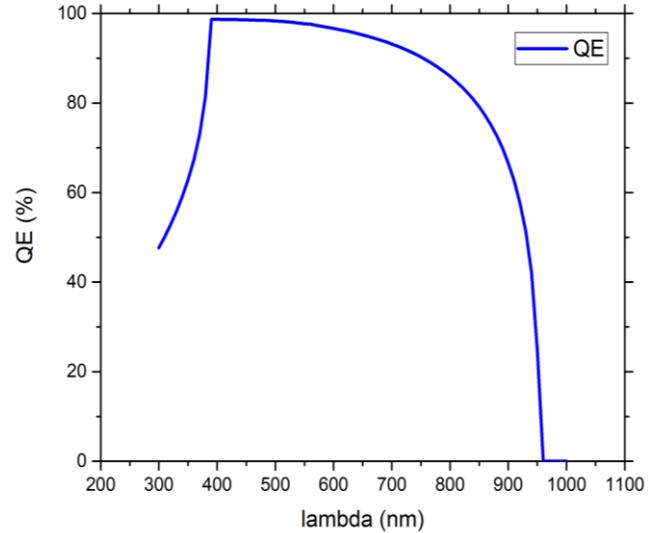


Figure 5. Quantum efficiency (QE) as a function of wavelength

Due to its narrower bandgap of 1.3 eV, the CH₃NH₃SnI₃ perovskite has an optical absorption edge that is shifted to 960 nm, as seen in the external quantum efficiency (QE) curve (Figure 5). The QE covers the entire visible spectrum and reaches a maximum absorption at 400 nm to nm, with notable absorption beginning at 960 nm. The red shift of the QE curve is advantageous for absorption of infrared wavelengths.

B. Effect of absorbent layer thickness

The absorbing layer plays a very important role in the performance of the cell, so to study this effect we varied the thickness of the absorbing layer from 100 nm to 1000 nm. The simulation results are shown in Figure 6. We can see that the variation of the thickness of the perovskite affects all the parameters of the cell. The current density (J_{sc}) increases with the increasing thickness of the absorber (perovskite), due to the large absorption coefficient of the latter. The PCE increases with the increasing thickness, reaching a maximum of 18,50 % at a thickness of 600 nm. Beyond this thickness, it begins to decrease due to the charge carrier diffusion length becoming shorter than the thickness of the perovskite, with some carriers not reaching the electrodes. The slight decrease in V_{co} with thickness is also due to an increase in recombination. The decrease in fill factor with increasing absorber thickness can be attributed to the increasing series resistance of the latter. This simulation study therefore confirms that the film must have an optimal thickness of 600 nm. This shows that perovskite is a material that, even with thicknesses of only a few hundred nanometres, is able to have better light absorption and higher efficiency.

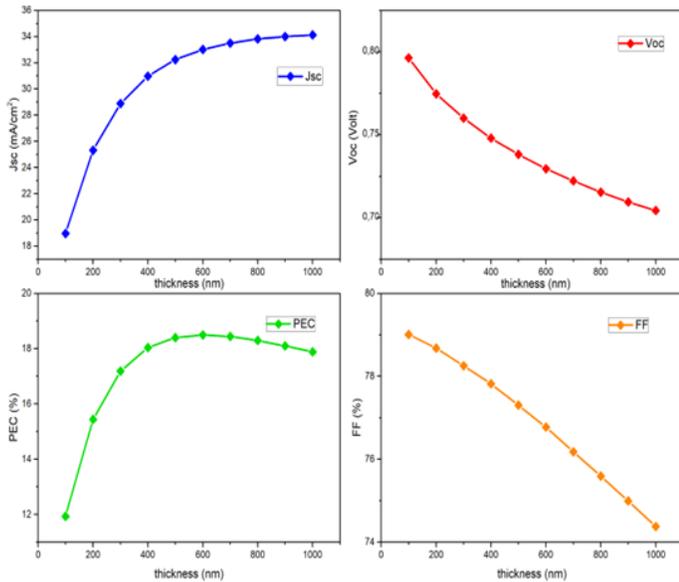


Figure 6. Variation of photovoltaic parameters as a function of $\text{CH}_3\text{NH}_3\text{SnI}_3$ thickness.

C. Effect of ETL layer thickness (TiO_2)

Here, it is observed that the thickness of the TiO_2 layer does not have an effect on all the cell's performance, so a thickness of 100 nm was chosen, based on comparison with values already published in the literature

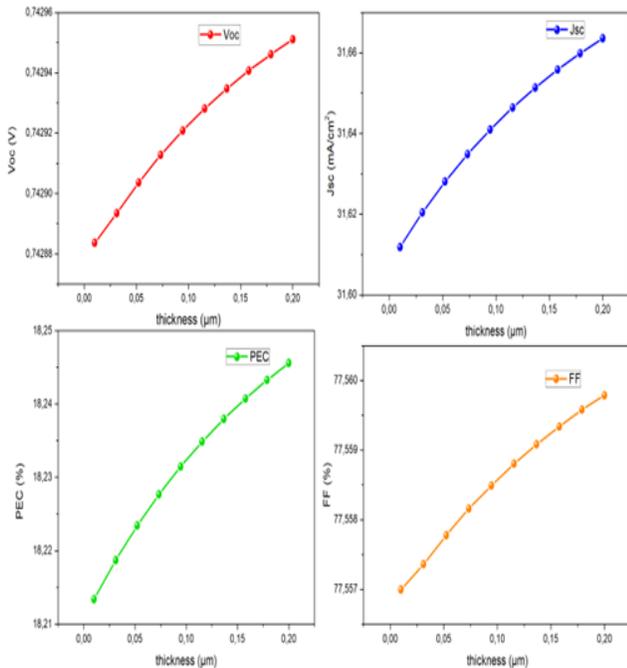


Figure 7. Variation of photovoltaic parameters as a function of TiO_2 thickness

D. Effect of HTL (Cu_2O) layer thickness

According to Figure 8, the thickness of the Cu_2O HTL layer has almost no effect on the generated photocurrent, but does affect the other parameters, only for very low values (less than 50 nm). Therefore, a value of 100 nm was chosen, in accordance with other references.

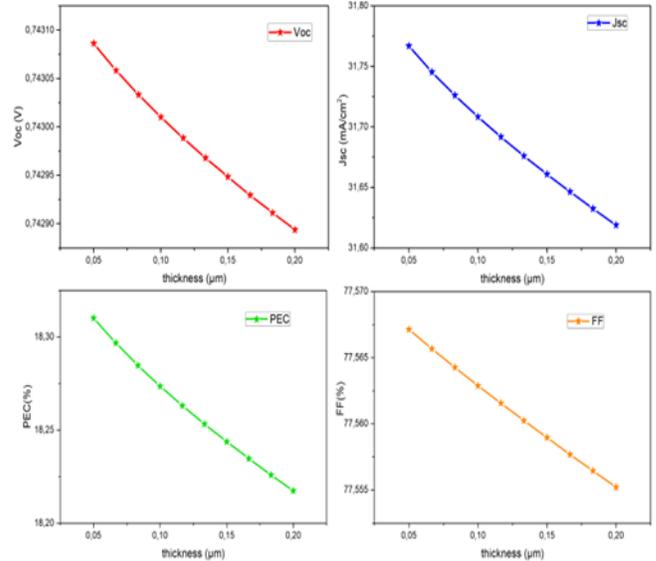


Figure 8. Variation of photovoltaic parameters as a function of Cu_2O thickness

E. Effect of the Na acceptor density (cm^{-3}) of the absorbing layer

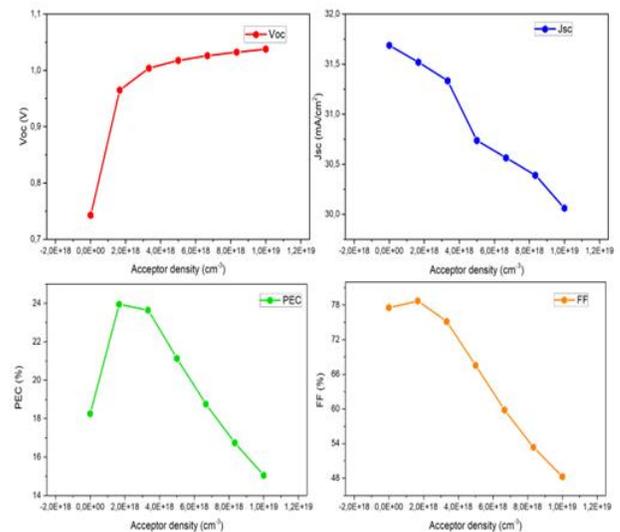


Figure 9. Variation of photovoltaic parameters as a function of Na acceptor density (cm^{-3}).



According to Figure 9, it can be seen that the cell's performance is only affected by the hole acceptor density above a value of 10^{15} cm^{-3} . A slight change in PV parameters is observed with increasing acceptor doping concentration up to $1,66675 \times 10^{18} \text{ cm}^{-3}$. V_{oc} increases as the Fermi energy of the holes decreases. Initially, J_{sc} decreases slightly and then decreases dramatically. This is likely due to an increase in charge carrier recombination within the perovskite absorbing layer [8]. However, PCE drops rapidly when Na exceeds $1,66675 \times 10^{18} \text{ cm}^{-3}$.

F. The photovoltaic parameters of the optimized cell

The final device features an absorbing layer thickness of 600 nm and a hole acceptor density of Na equal to $1,67 \times 10^{18} \text{ cm}^{-3}$. The photovoltaic parameters of both the reference cell and the optimized $\text{CH}_3\text{NH}_3\text{SnI}_3$ -based cell are reported in Table 3. It is clear from the results that the optimized cell exhibits significantly improved performance compared to the reference cell. This demonstrates the importance of carefully considering and manipulating various device parameters during the optimization process in order to achieve high-efficiency photovoltaic devices. The results also highlight the effectiveness of the optimization efforts in achieving this goal. Overall, this study emphasizes the critical role of device design and optimization in the development of high-performance solar cells.

Table 3.
Photovoltaic parameters of the reference and optimized cell.

	V_{oc} (V)	J_{sc} (mA/cm ²)	FF (%)	PCE (%)
Reference cell	0,748	30,982	77,819	18,035
Optimized cell	0,965	31,519	78,717	23,943

IV. CONCLUSION

In conclusion, we have studied and simulated a solar cell based on the perovskite material $\text{CH}_3\text{NH}_3\text{SnI}_3$ using the one-dimensional simulation tool SCAPS-1D. Our main objective was to determine the optimal parameters to improve the performance of the solar cell. Our simulation results show that the thickness, doping concentration, work function, defect density of the absorbing layer, and defects at the interfaces play a significant role in the performance of the solar cell.

After optimizing the photovoltaic parameters of the absorbing layer, we were able to significantly improve the electrical performance of the solar cell. Specifically,

we achieved a J_{sc} of 31.52 mA/cm^2 , a V_{oc} of 0.97 V, an FF of 78.72%, and a PCE of 23.95%. These findings demonstrate the effectiveness of optimization efforts in achieving high-performance solar cells and highlight the importance of considering various device parameters in the design process.

In summary, our study provides important insights into the design and optimization of perovskite solar cells. Our findings could guide future efforts to develop more efficient and cost-effective solar cell technologies, which are crucial for the widespread adoption of renewable energy sources and the mitigation of climate change.

CONFLICTS OF INTEREST

The authors declare that there is no conflict of interest.

RESEARCH AND PUBLICATION ETHICS

In the studies carried out within the scope of this article, the rules of research and publication ethics were followed.

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