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Simulation-Based Optimization of the Performance of a $CsPbI_3$ (Cesium Lead Triiodide) Perovskite Solar Cell Using SCAPS-1D

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Abstract

In this work, we report a simulation optimization of the performance of a perovskite solar cell using the SCAPS-1D simulation program. We analyzed the influence of the perovskite layer thickness, as well as the thickness of the electron transport material (ETM) and hole transport material (HTM) layers, the concentration of Na acceptors, and the influence of other HTM materials on the performance of the $CsPbI_3$ cell. The results acquired in simulation show that this type of perovskite solar cells can achieve a theoretical conversion efficiency of 24.2% at room temperature, with an open-circuit voltage of $V_{oc} = 1.45$ V, a short-circuit current density of $J_{sc} = 20.51$ mA/cm^2, and a form factor of FF = 81.57%. The validity of the proposed perovskite ($CsPbI_3$) cell is proven by comparing its results with the recently published results, where the efficiency reached 19.1% in 2022, theoretically by M. Khalid Hossain and his collaborators and 18.4% experimentally in 2019 by Y. Wang and his collaborators. The efficiency we obtained is one of the highest power conversion rates compared to the recently published results. Considering these results, $CsPbI_3$-type perovskite solar cells present a good compromise between conversion efficiency and manufacturing cost and can thus enable potential applications in large areas.

Keywords

Simulation, Performances, Perovskite, $CsPbI_3$, SCAPS-1D, Optimization

1. Introduction

The direct conversion of sunlight into electricity is possible thanks to the technique of photovoltaic solar energy. This method is based on the use of photovoltaic cells, known as solar modules, which capture the photons present in sunlight and transform them into electric current [1].

Photovoltaic energy is considered a clean and renewable energy source because it does not generate greenhouse gases or air pollution during its operation. It offers many advantages, such as durability, reliability, and ease of deployment. Solar cells are composed of photovoltaic cells that are usually made from semiconductors such as silicon. These semiconductors have the property of producing an electric current when exposed to light. Solar modules can be installed on roofs, ground support structures, or integrated into portable devices. When sunlight hits the photovoltaic cells, the photons excite the electrons present in the semiconductor material, creating a direct electric current [2]. This current can be used directly to power electrical devices or stored in batteries for future use.

In recent decades, photovoltaic technology has experienced considerable growth, characterized by constant improvements in solar cell efficiency, reduced production costs, and an increase in global production capacity. Photovoltaic installations have become widespread both on a large scale in solar parks and on a small scale on the roofs of houses and buildings, thus contributing to the energy transition by offering an alternative to traditional energy sources such as coal, natural gas, and oil [3]. This technique has enormous potential to sustainably meet global energy needs by reducing dependence on fossil fuels and contributing to global warming.

However, even though photovoltaic solar energy offers many benefits, it still faces some challenges. These challenges include energy storage, grid integration, and recycling of solar panel materials at the end of their life. However, despite these obstacles, photovoltaic technology continues to advance and improve, paving the way for a cleaner and more sustainable energy future.

Perovskite solar cells (PSCs) are considered the future of photovoltaic technology, as they are capable of generating power conversion efficiency close to that of the main silicon solar cells [4], while being less expensive. Their enormous potential lies in their efficiency progression, increasing from 3.8% to 25.2% in a decade, with a continuous increase to date. The selection of perovskite composition plays a vital role in achieving optimal performance. In this work, efforts are made to study lead-containing perovskite solar cells to improve their performance.

2. Materials and Methods

2.1. Cell Structure

The manufacturing of perovskites is a complex process; therefore, the scientific community mainly relies on simulation tools for material optimization. For this purpose, various simulation tools such as wx-AMPS, SCAPS-1D, Silvaco-TCAD, etc. are available online for research and design, but we have used SCAPS-1D in this work.

$CsPbI_3$ was selected because of its thermal stability due to its band gap of 1.73 eV, it has a wide absorption range of sunlight, which allows it to capture a large part of the solar spectrum and this property is essential for efficient conversion of solar energy into electricity. However, it is well known that $CsPbI_3$ suffers from phase instability at room temperature, often transforming from the black perovskite (α) phase to the yellow non-perovskite (δ) phase. This instability indeed limits its long-term operational stability. Nevertheless, our choice of $CsPbI_3$ is motivated by its wide band gap (1.73 eV), all-inorganic composition (free from organic cations such as MA^+ or FA^+), and potential for high thermal stability when stabilized via compositional or interfacial engineering, as reported in recent studies [5] [6]. Therefore, our simulation focuses on its intrinsic photovoltaic potential under idealized stable conditions. Its structure is shown in **Figure 1**.

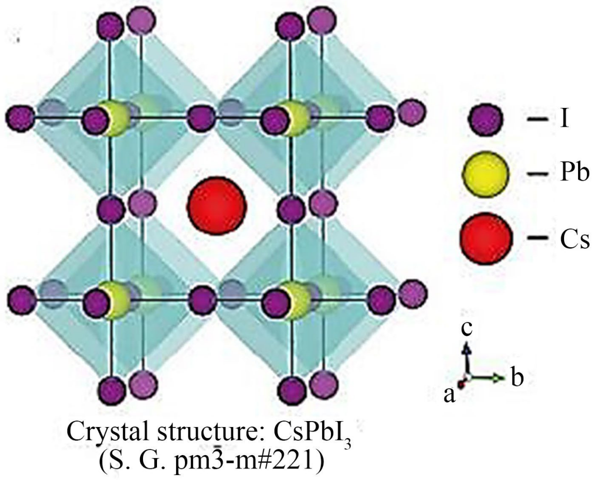

Figure 1. Crystal structure of $CsPbI_3$.

2.2. Cell Parameters Used in the Simulation

Before starting the simulation, it is essential to have prior knowledge of certain parameters of each layer of the cell. **Table 1** and **Table 2** group together the parameters of the different materials used for the simulation. All material parameters, such as bandgap, mobility, and carrier densities, were taken from peer-reviewed literature [7]-[11] without manual fitting, ensuring that the simulated device structure reflects realistic material properties reported experimentally.

Table 1. Parameters of each cell layer used for simulation

Settings	ZnO (ETM)	$CsPbI_3$	PTAA (HTM)
Thickness W (nm)	25	450	50
Gap energy E_g (eV)	3.3	1.73	2.96
Electron affinity χ (eV)	4	3.96	2.3
Relative permittivity ε_r	9	10	9

Continued

Conduction band N_c (cm^{-3})	2.2×10^{15}	2×10^{14}	1×10^{15}
Valence band N_V (cm^{-3})	1.8×10^{15}	5×10^{14}	1×10^{15}
Thermal velocity of electrons (cm/s)	10^7	10^7	10^7
Thermal velocity of holes (cm/s)	10^7	10^7	10^7
Electron mobility μ_n (cm^2/Vs)	100	20	1
Hole mobility μ_p (cm^2/Vs)	25	20	40
Effective donor density N_D (cm^{-3})	1×10^{15}	1×10^{20}	0
Effective density of acceptors N_A (cm^{-3})	0	1×10^{20}	1×10^{15}
Reference	[7]	[8]	[9]

Table 2. HTM layer parameters.

Settings	PEDOT:PSS	CuSCN
Thickness W (nm)	50	150
Gap energy E_g (eV)	1.6	3.4
Electron affinity χ (eV)	3.4	1.9
Relative permittivity ε_r	3	10
Conduction band N_c (cm^{-3})	2.2×10^{18}	1.7×10^{19}
Valence band N_V (cm^{-3})	1.8×10^{19}	1.8×10^{19}
Thermal velocity of electrons (cm/s)	10^7	10^7
Thermal velocity of holes (cm/s)	10^7	10^7
Electron mobility μ_n (cm^2/Vs)	4.5×10^{-2}	2×10^4
Hole mobility μ_p (cm^2/Vs)	4.5×10^{-2}	2×10^1
Effective donor density N_D (cm^{-3})	0	0
Effective density of acceptors N_A (cm^{-3})	10^{18}	1.01×10^{18}
Total defect density N_T (cm^{-3})	10^{15}	10^{14}
Reference	[10]	[10]

Table 1 shows the input parameters of ETM, HTM of the absorber layer. On the other hand, Table 2 groups the HTM parameters for the second part of the simulation in order to find a perfect combination. In addition, all simulations were carried out using the conditions of the AM1.5G solar spectrum, which is equivalent to a power density of 1000 Wm^2 at 300 K ambient temperature.

PEDOT:PSS and CuSCN are two commonly used materials in perovskite solar cells due to their specific advantages. PEDOT (poly(3,4-ethylenedioxythiophene)) and PSS (poly (styrene sulfonate)) (PEDOT:PSS). These two materials refer to a mixture of two conductive polymers, This mixture is used in many electronic and optical applications due to its high conductivity and transparency properties, which facilitates the transport of electrical charges generated by the perovskite to the electrodes of the solar cell, good transparency that allows light to reach the perovskite and generate charges and facilitates the alignment of energy levels between the perovskite and the electrode, thus improving the efficiency of charge collection.

CuSCN (copper thiocyanate) is a chemical compound consisting of copper ions (Cu^{2+}) and thiocyanate ions (SCN^-), often used as a semiconductor material in some electronic devices and as a catalyst in certain chemical reactions. It is a chemically stable material, which is important for the long-term durability of perovskite solar cells and offers simpler and potentially lower manufacturing costs.

3. Results and Discussions

3.1. Study of the Variation of the Thicknesses E (µm) of the Layers on the Characteristics of the Cell

3.1.1. Effect of the Thickness E (µm) of the PTAA Layer (HTM)

In this study, we also modulated the thickness of PTAA (hole transport layer) *Poly* (*triarylamine*) (*PTAA*) instead of just *PTAA*, in a variation range of 50 nm to 300 nm to determine the optimal thickness of the HTM material by fixing the other parameters constant. Figure 2 presents the effect of this thickness variation on the performance of the solar cell. We note that as the thickness of this layer varies, the conversion efficiency η, the short-circuit current density and the open-circuit voltage remain almost constant, and we observe a slight decrease in the form factor FF from 0.05 µm to 0.15 µm before being constant up to 0.30 µm.

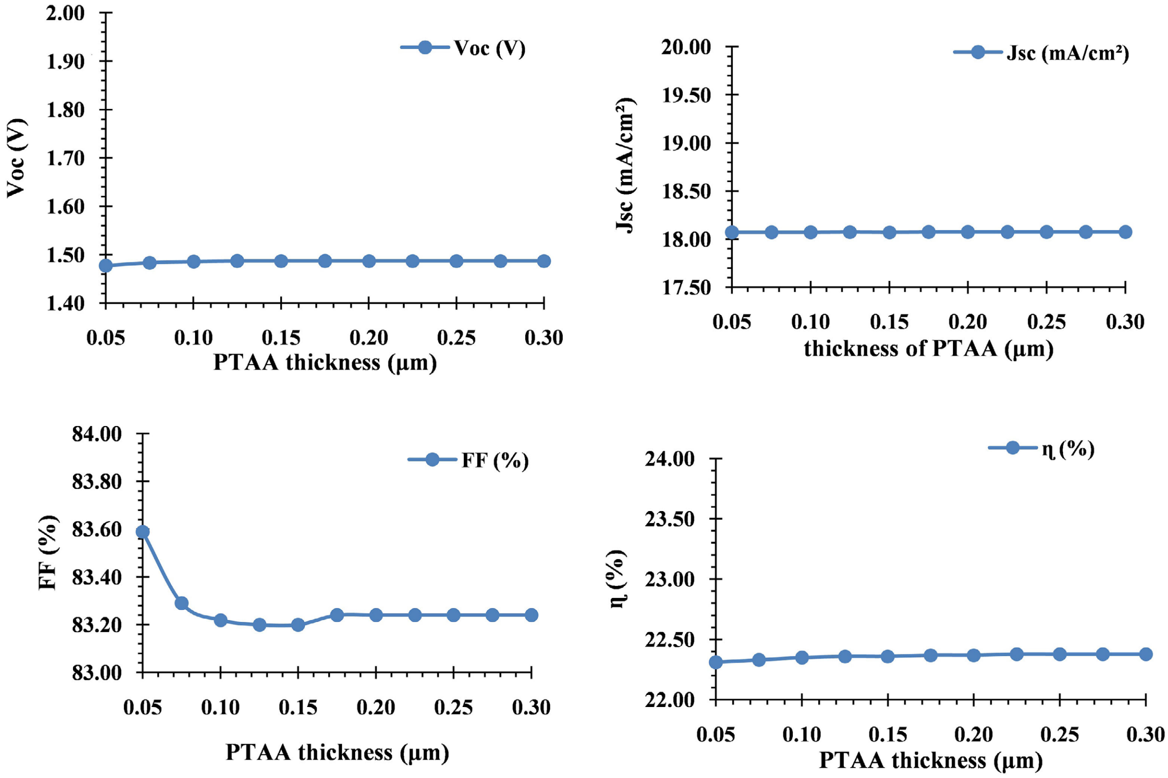

Figure 2. Variation of HTM layer thickness as a function of cell characteristics.

After extensive analysis, we determined the optimal HTM thickness to be 50 nm, which was consistent with the initial setting of our study. In a solar cell structure, the p-type layer (HTM) should generally be thicker than the n-type layer (ETM). This helps reduce the probability of charge recombination by facilitating the rapid transport of an equal number of charge carriers to their respective terminals [11]. Furthermore, a larger thickness for the HTM has additional benefits, as it improves the ability of the light-collecting layer to absorb photons.

3.1.2. Effect of the Thickness W (μm) of the ETM Layer

ZnO layer thickness (ETM), changing it from 20 nm to 200 nm, while the other parameters were kept constant. Figure 3 presents the results of this variation of the ETM thickness and illustrates the effect of this variation on the performance parameters of the solar cell. From 0.02 to 0.2 μm, we observe a decrease in the short-circuit current density J_{sc} (mA/cm^2) from 18.075 to 18.019 mA/cm^2 or a rate of 0.3%; as well as for the form factor of 84.00% at 83.08% or a rate of 1.1% and the conversion efficiency η (%) of 22.32 to 21.99 or a rate of 1.5%, on the other hand the open circuit voltage remains constant V_{oc} (V).

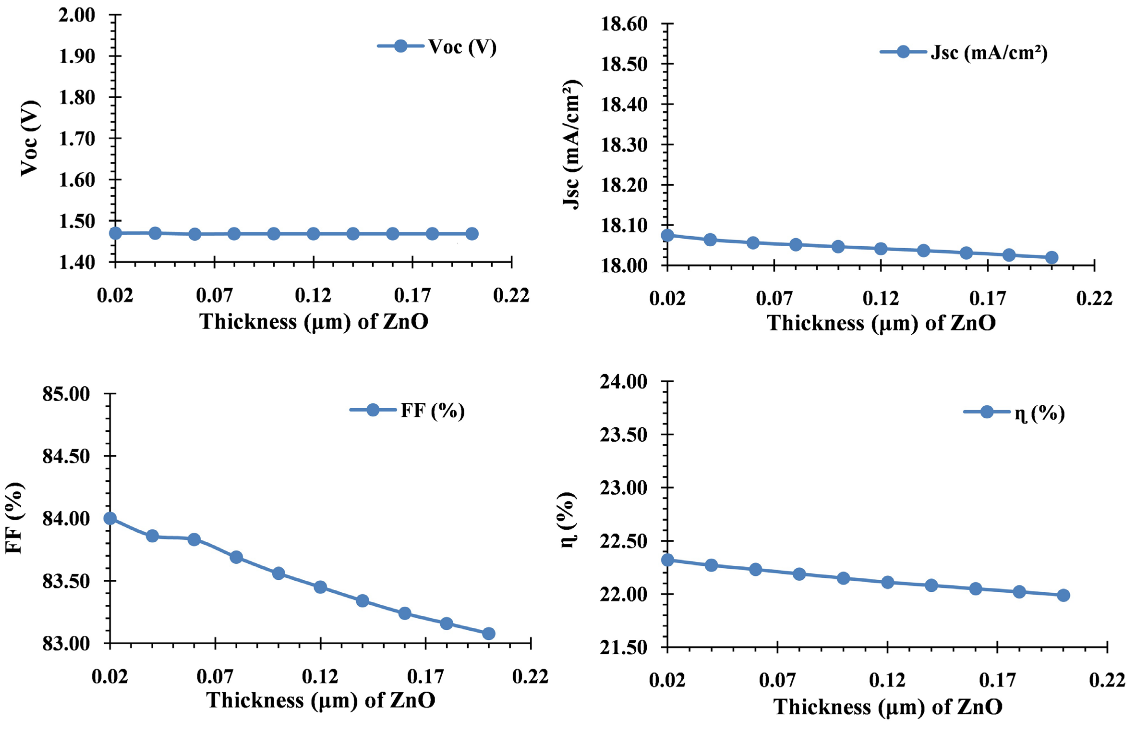

Figure 3. ZnO thickness depending on cell characteristics.

Increasing the ETM thickness resulted in lower values of V_{oc}, J_{sc}, FF and η, although this decrease was insignificant. This observation can be attributed to the fact that thicker ETM partially absorbs light, thus delaying charge generation and electron collection rate. As the ETM becomes thicker, the performance loss becomes more pronounced due to the decrease in light transmission [10]. ZnO was selected as the electron transport material due to its high electron mobility, suitable band alignment with $CsPbI_3$, and low-temperature processability. While TiO_2 is more commonly used, ZnO offers better conduction properties and can reduce interfacial recombination when properly passivated. Comparative results in Section 3.3 confirm its superior performance in this configuration.

However, it is important to emphasize that, according to our results, the thickness of the ETM had a limited impact on the photovoltaic performance of the solar cell, which is consistent with previous work [11]. Therefore, a thickness of 20 nm was identified as the best thickness for ETM in this study.

3.1.3. Effect of the Thickness E (μm) of the $CsPbI_3$ Absorbing Layer

For this part, we study the cell characteristics as a function of the thickness of the absorbing layer, which varies from 200 nm to 1100 nm, keeping the other parameters constant. The optimal thickness of the absorbing layer is crucial to maximizing photon absorption and generating electron-hole pairs.

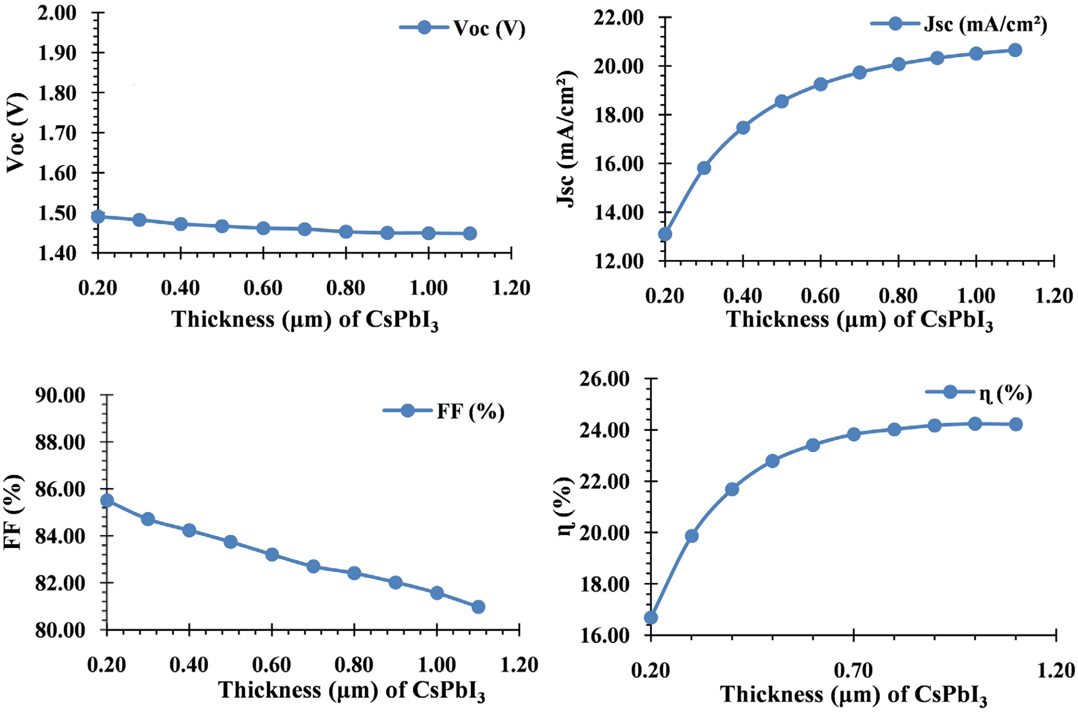

Figure 4. Variation of the thickness (μm) of the perovskite depending on the characteristics of the cell.

Therefore, the overall performance of the solar cell mainly depends on the thickness of the absorber layer. The graphs shown in **Figure 4** illustrate the variations of the open-circuit voltage (V_{oc}), the short-circuit current density (J_{sc}), the fill factor (FF) and the efficiency (η) as a function of the thickness of the perovskite layer, respectively.

According to the simulation results, we notice that when the thickness of the active layer increases, there is a decrease in the open circuit voltage (V_{oc}) from 1.49 V to 1.45 V or a rate of 2.7% and the form factor (FF) which goes from 85.51 to 80.98 or a rate of 5.3%, on the other hand we have an increase in the short-circuit current density (J_{sc}) from 13.10 mA/cm^2 to 20.65 mA/cm^2 or a rate of 57.6% and the conversion efficiency (η) from 16.70% to 24.24% it reaches this percentage at 1µm of the thickness, after this value it undergoes a fall.

By increasing the thickness of the active layer, the current density (J_{sc}), open-circuit voltage and efficiency increase because a thicker absorber layer will absorb more photons, which will create many more excitons and allow the generation of electron-hole pairs.

But with too thick an absorbing layer, the chances of recombination also increase because the generated photocharges have to travel a greater distance to be diffused [12]. This increased absorption helps increase the efficiency of the solar cell by capturing more photons for the generation of electron-hole pairs.

3.2. The Effect of Doping Concentration (Na) of PTAA (HTM)

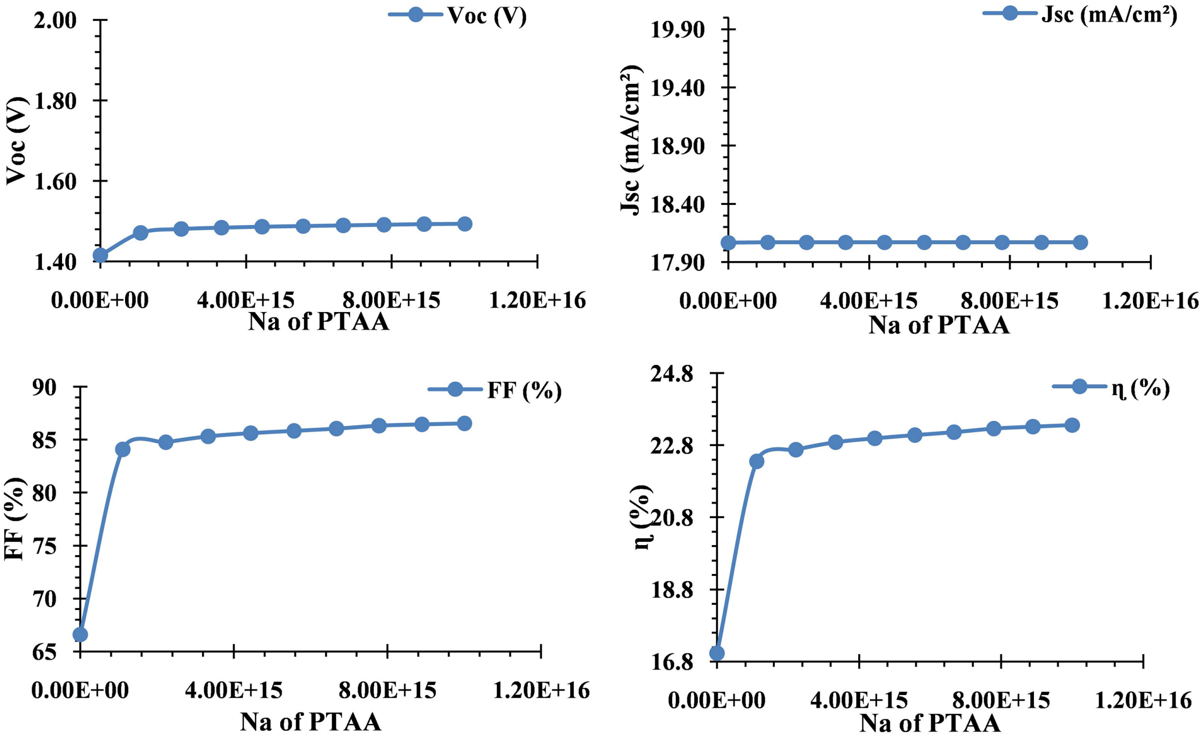

Figure 5. Variation of PTAA acceptor concentration (Na) as a function of cell characteristics.

In this study, the Na doping of PTAA is considered as a theoretical assumption used to explore how the modification of acceptor density in the HTM layer influences cell performance. In practice, alkali-metal incorporation in organic HTMs remains challenging; however, recent works have reported partial ionic doping or surface treatment approaches that modify energy levels or improve hole extraction. Our approach, therefore, aims to provide an initial numerical insight rather than a confirmed experimental process. Doping is a very important process used to improve the photovoltaic properties of semiconductors, it influences the electrical behavior of the layers and thus affects the cell performance. **Figure 5** shows the effect of Na of PTAA on the open circuit voltage V_{oc}, short circuit current J_{sc}, form factor FF and conversion efficiency η of the PSC when varied from 10^{12} cm^{-3} to 10^{16} cm^{-3}, and we notice an increase in all the parameters.

This increase in electrical potential creates a separation of excitons with a lower recombination rate, which increases the performance of the cell. It promotes conductivity, thus facilitating the transport of holes to the anode, while reducing the defect and impurity density in the layer.

3.3. Effect of HTM

This part aims to find a HTM material that performs better than the organic PTAA material that allowed us to obtain 24.24% efficiency. So, we will fix the other parameters of the perovskite and keep ZnO as the ETM because it has the best performance compared to other ETMs, and it is therefore the best ETM for the $CsPbI_3$ absorbing layer [13]. We will use two other HTM materials, PEDOT:PSS and CuSCN (see **Figure 6**).

- For PEDOT:PSS

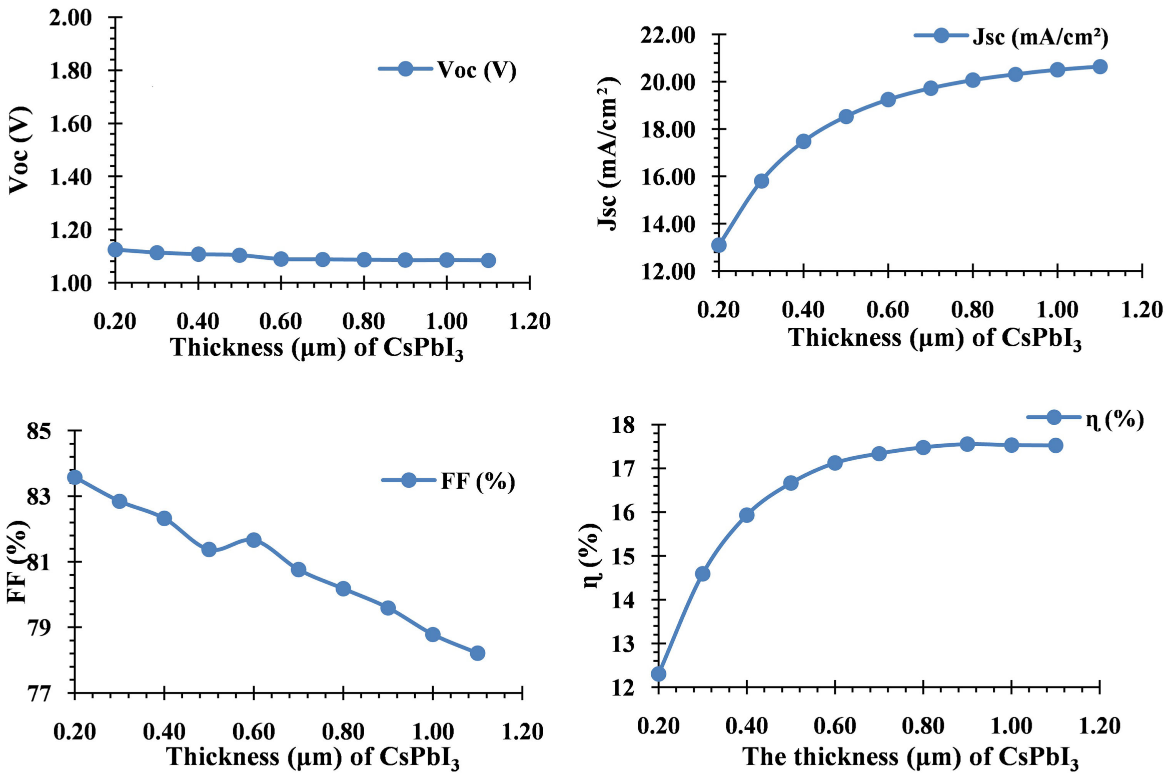

Figure 6. Variation of the perovskite layer thickness with PEDOT:PSS as HTM as a function of the cell characteristics.

- For CuSCN

We summarize (**Table 3**) the performance obtained after the use of different hole transport material, both fixing the active layer ($CsPbI_3$) and the layer of electron transport material (ZnO) (see **Figure 7**).

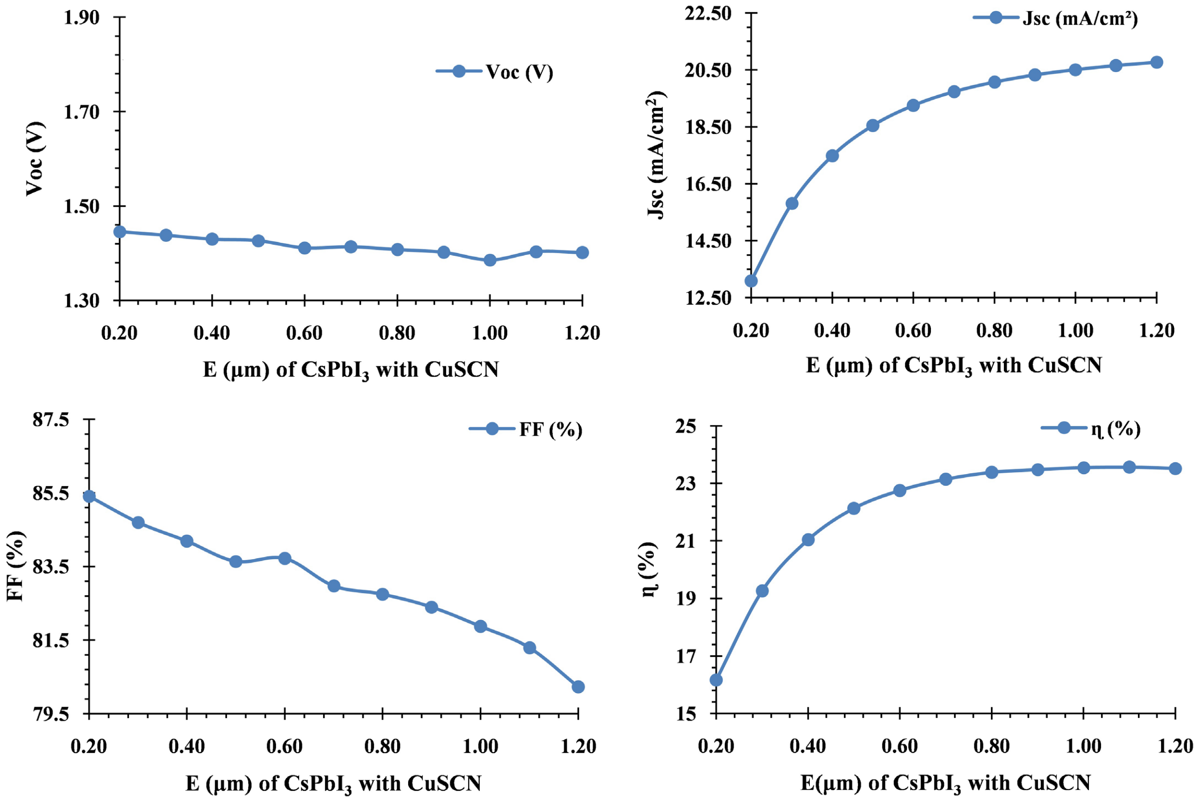

Figure 7. Variation of the thickness of the perovskite layer with CuSCN as HTM.

Table 3. Simulation results of the performance of each HTM.

	PEDOT:PSS	CuSCN	PTAA
Thickness (μm) of $CsPbI_3$	0.90	1.00	**1.00**
V_{oc} (V)	1.08	1.39	**1.45**
J_{sc} (mA/cm^2)	20.32	20.51	**20.51**
FF (%)	79.60	81.87	**81.57**
PCE (%)	17.55	23.55	**24.24**

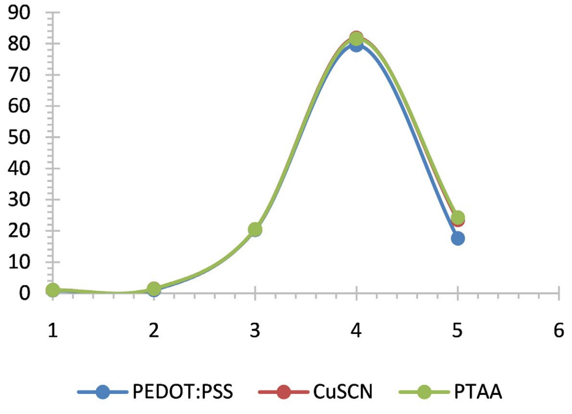

Figure 8. The performance of each HTM layer.

After the simulation of the two materials, we notice that the results of the materials are almost similar, but CuSCN has better performance than PEDOT:PSS, but we retain that PTAA remains the best HTM material for a $CsPbI_3$ absorbing layer (see **Figure 8**).

3.4. Comparison with Published Results

Table 4 shows the comparative analysis of recent experimental and theoretical work on $CsPbI_3$-based perovskites with our results. The SCAPS-1D model used here does not include explicit interface defect layers or surface recombination velocities. While this simplification allows for a clearer evaluation of bulk-layer effects, it may slightly overestimate the simulated efficiency compared to experimental data.

Table 4. The comparison of PV parameters of different solar cells based on $CsPbI_3$.

Reference	Year	Structure	Kind	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	η (%)
[14]	2018	$TiO_2/CsPbI_3$/PTAA	Exp.	1.20	15.25	78.70	14.50
[15]	2019	$TiO_2/CsPbI_3$/Spiro	Exp.	1.11	20.23	82.00	18.40
[16]	2021	$ZnO/CsPbI_3/CuSbS$	Theory	1.10	22.59	62.60	15.60
[13]	2022	$TiO_2/CsPbI_3$/CBTS	Theory	1.00	21.08	86.60	19.10
This work	**2023**	**$ZnO/CsPbI_3$/PTAA**	**Theory**	**1.45**	**20.51**	**81.57**	**24.24**

We note that the efficiency reached 19.1% in 2022 theoretically and 18.4% experimentally in 2019. As the results were not up to expectations in most theoretical studies, we tried to optimize the performance of this perovskite, and our results were the best, with an efficiency of 24.2%. It should be noted that the present simulation does not explicitly account for defect states at interfaces, ion migration phenomena, or long-term phase degradation, which are known to affect the real-world stability of perovskite devices. These aspects will be considered in future work using defect-layer and time-dependent modeling to enhance the physical accuracy of the simulation.

4. Conclusion

In this chapter, we studied and simulated the solar cell based on the perovskite material $CsPbI_3$ to extract the different parameters: J_{sc}, V_{oc}, FF and η using the SCAPS-1D simulation tool. The main objective is to improve the performance of the solar cell by determining the optimal parameters. Although this work is purely simulation-based, an experimental validation is planned in a subsequent study to fabricate $CsPbI_3$-based devices and compare measured parameters (V_{oc}, J_{sc}, FF, η) with the simulated trends. Simulation results showed that the thickness, doping concentration, defect density of the absorber layer and changing the HTM play an important role in the performance of the solar cell. The results obtained after optimizing the photovoltaic parameters of the absorber layer are (V_{oc} = 1.45 V, J_{sc} =

20.51 mA/cm^2, FF = 81.57%, η = 24.24%). These results show that the $CsPbI_3$ perovskite cell has better electrical performance.

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Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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