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Research Article

Exploring the Efficiency of $CH_3NH_3SnBr_3/CsPbI_3$ Heterojunction Solar Cell using Numerical Simulation

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Abstract – This study presents a numerical analysis of heterojunction perovskite solar cells (PSCs) with a proposed structure of Glass/ETL/i-$CH_3NH_3SnBr_3/CsPbI_3$/HTL using the SCAPS-1D software. The primary objective is to investigate the influence of the thickness of $CsPbI_3$ perovskite active layers with i-$CH_3NH_3SnBr_3$ as the permeable layer. Additionally, the power conversion efficiency (PCE), temperature dependence, quantum efficiency, open-circuit voltage (Voc), fill factor (FF), short-circuit current density, and J-V curve simulations for varying Na are examined. The highest PCE achieved was 42 %, accompanied by an FF of 90 %, Voc of 1.29 V, and Jsc of -35,42 mA/cm^2. The findings of this analysis contribute to the understanding of the performance and optimization of heterojunction perovskite solar cells, highlighting the significance of layer thickness and device parameters in achieving high-efficiency solar energy conversion.

Keywords – Heterojunction Perovskite, SCAPS-1D, $CsPbI_3$, i-$CH_3NH_3SnBr_3$.

I. INTRODUCTION

Perovskite-based solar cells have gained a lot of attention in recent years due to their potential for high efficiency and low-cost production. The achievement by researchers at the Helmholtz Zentrum Berlin (HZB) in achieving a solar cell that transforms 32.5% of incoming solar radiation into electrical energy is indeed a significant milestone and sets a new global record. Perovskite solar cells are a type of thin-film solar cell that uses a material with a perovskite crystal structure as the light-harvesting layer. This structure allows for efficient absorption of a wide range of solar wavelengths. Perovskite materials can be processed using low-cost methods, such as solution processing, which makes them attractive for large-scale production. The high efficiency achieved by the researchers at HZB is a remarkable advancement for perovskite solar cells. High-efficiency solar cells are crucial for maximizing the energy conversion from sunlight, which can lead to more cost-effective and sustainable solar energy systems.It's important to note that while this achievement is promising, further research and development are needed to address challenges associated with stability, durability, and scalability of perovskite solar cells. These factors are crucial for commercial viability and widespread adoption of this technology. Nonetheless, this breakthrough by HZB researchers highlights the continuous progress being made in the field of perovskite-based solar cells and brings us closer to more efficient and affordable solar energy solutions [1].

In this study, we have proposed $CuSbS_4$ as a layer for transporting holes(HTL) holes ,where the HTL plays a crucial role in the efficient extraction of

charge carriers and improving the overall device performance.$CuSbS_4$ is a semiconductor material with suitable energy levels and hole mobility, making it suitable for use as an HTL,it has been investigated for applications in solar cells[2], where it can be employed as an HTL to transport holes from the light-absorbing layer (typically a perovskite or other light-absorbing material) to the electrode and we chose to work with two types of perovskite. Firstly, the i-$CH_3NH_3SnBr_3$ which belongs to the hybrid halide perovskites p-type. It pertains to a semiconductors class with general formula ABX_3; in which the metal cation B, is Sn^{2+}, in the center; X represents a mono-valent anion Br^-; and A is monovalent cation, such as the organic molecular $[CH_3NH_3]^+$, chosen to neutralize the overall charge [3]. Secondly, the inorganic halide perovskites $CsPbI_3$ were reported to show higher thermal stability [4,5]; especially, the inorganic perovskites, $CsPbI_3$ with the cubic phase which exhibits the most suitable bandgap of 1.73 eV for photovoltaic applications [6,7]. From 2015 until now, the device efficiency for $CsPbI_3$ has enhanced from 2.9% [6,8] to 19.03% [9] together with improved stability, indicating its great potential for high-efficiency inorganic PSCs. Titanium dioxide (TiO_2) is commonly used as an electron transport layer (ETL) in various types of solar cells, including perovskite solar cells and dye-sensitized solar cells (DSSCs).

TiO_2 is a wide band gap semiconductor, meaning it has a large energy difference (Eg) between its valence band and conduction band. The band gap of TiO_2 is typically around 3.26 eV, which makes it suitable for absorbing high-energy photons from the solar spectrum. In perovskite solar cells, TiO_2 is often used as the electron transport layer that collects and transports the photo-generated electrons from the perovskite layer to the electrode. It provides a favorable energy level alignment for efficient charge extraction and also helps to prevent recombination of electron-hole pairs. The combination of TiO_2 with its unique properties and its compatibility with other materials makes it a widely used and successful component in perovskite and dye-sensitized solar cells [10,11].

II. Materials and Method

The proposed heterojunction used in this work is Glass/ETL/i-$CH_3NH_3SnBr_3$/$CsPbI_3$/HTL/ are depicted in Fig 1.

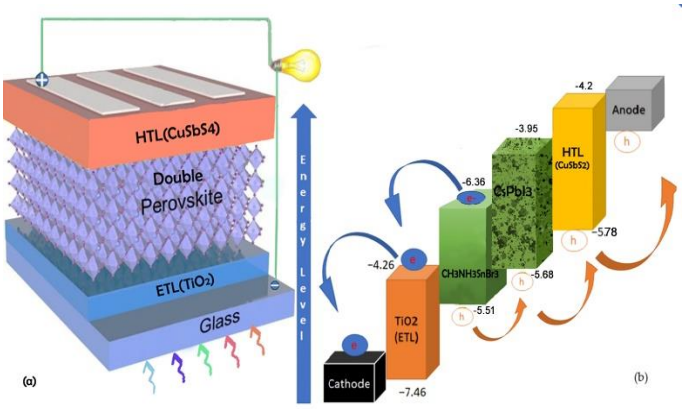

Fig 1 : (a) Schematic structure view (b) Energy level diagram of ETL/ i-$CH_3NH_3SnBr_3$/ $CsPbI_3$/HTL heterojunction solar cell.

The numerical simulation of solar cells is used by SCAPS-1D which was programmed by Burgelman at the university of Gent, Belgium [12], and it is about a software package used for simulating the behavior and performance of thin-film solar cells, is primarily used by researchers and engineers in the field of photovoltaics to model and analyse the electrical and optical properties of various types of solar cells. The software is based on a one-dimensional simulation approach, which simplifies the modelling process by assuming that the properties of the solar cell are uniform in one direction. It takes into account various physical phenomena, such as carrier transport, generation, recombination, and optical absorption, to accurately predict the performance of solar cells under different operating conditions.

Users can input material parameters, device geometries, and environmental conditions into SCAPS-1D to simulate and analyse the electrical characteristics (such as current-voltage curves, power conversion efficiency, and capacitance-voltage characteristics) of solar cells. The software provides detailed outputs, including internal device profiles, carrier densities, and electric field distributions, which help in understanding the device physics and optimizing the solar cell design.

In the simulation of the photovoltaic cell under illumination, several parameters and conditions were taken into account. The thermal velocity of electrons and holes used in the simulation was 10^7 cm/s. This parameter represents the average velocity of charge carriers (electrons and holes) due to thermal energy at a given temperature.

The standard photovoltaic radiation spectrum AM 1,5G was employed, which represents the solar spectrum under terrestrial conditions. It has a power density of 1000 W/m^2 and a temperature of 300 K.

This spectrum is widely used in photovoltaic simulations to evaluate the performance of solar cells. The thickness of the ETL (Electron Transport Layer) layer in the solar cell was fixed at 0,1 µm. Similarly, the thickness of the HTL (Hole Transport Layer) was set at 0.05 µm. The HTL is responsible for facilitating the movement of positive charges (holes) in the solar cell structure. To perform the simulations, various material parameters were considered, and they are summarized in Table 1. These parameters define the properties of the materials used in the solar cell, such as their electronic structure, conductivity, mobility, and recombination rates. By specifying these material parameters, the simulation can accurately represent the behavior and performance of the solar cell under different conditions.

Table 1 regroup the physical parameters employed in our simulation.

	HTL	$CsPbI_3$	$CH_3NH_3SnBr_3$	ETL
Layer thickness (nm)	50	Varied	Varied	100
Dielectric constant dk	14.6	6	10.000	10.000
Band gap Eg (eV)	1.58	1.690	1.3	3.260
Electron affinity chi (eV)	4.2	3.590	4.170	4.200
Effective conduction band density (cm^{-3})	2.5E+10^{18}	1.10^{20}	2.200E+18	1E+10^{21}
Effective valence band density (cm^{-3})	1E+10^{19}	8.20^{20}	1.800E+18	2E+10^{20}
Electron mobility (cm^2 V^{-1} s^{-1})	49	25	1.6	10
Hole mobility (cm^2 V^{-1} s^1)	4.9E+10^9	25	1.6	25
Doping concentration of donators (cm^{-3})	0	0	1E+10^{13}	1E+10^{19}
Doping concentration of acceptors (cm^{-3})	1.38 E+10^{18}	1E+10^{15}	1×10^{13}	0
Thermal velocity of electron (cm^{-3} s^{-3})	1E+10^7	1E+10^7	1E+10^7	1E+10^7
Thermal velocity of holes (cm^{-3} s^{-3})	1E+10^7	1E+10^7	1 E+10^7	1E+10^7
References	[13]	[14]	[15]	[16]

III. RESULT AND DISCUSSION

A. Optimization of absorber layer thickness

In the mentioned section, the thickness of the absorber layer, specifically the perovskite layer, is being varied in order to optimize its performance. The range of thickness variations explored for the absorber layer is from 0.1 µm to 3 µm.

It's important to note that the thickness of the ETL and HTL layers is kept fixed at their initial values during this optimization process. After varying the thickness of the $CH_3NH_3SnBr_3$ layer (from 0.1 um to 3 um) and the CsPbI3 layer (also from 0.1 um to 0.9 um), the thickness value that yields the best power conversion efficiency (PCE) is determined.

Once the optimal thickness value for the absorber layer is identified, it is then fixed and used for the remaining parts of the paper or study. By fixing this thickness, researchers can ensure consistent and reliable performance measurements and comparisons throughout their research.

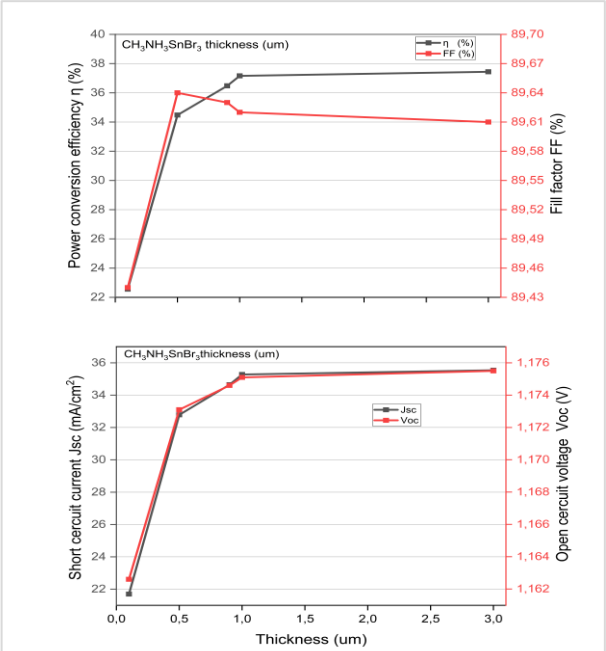

Fig 2 :The influence of $CH_3NH_3SnBr_3$ thickness on the properties of solar cell.

The Fig 2 the relationship between the thickness of the $CH_3NH_3SnBr_3$ layer and the performance of solar cells; Notably, it is noted that the greater the thickness the better the efficiency, which rises from 22.56% to 37%, this observation suggests that the thickness of the $CH_3NH_3SnBr_3$ plays a significant role in enhancing the performance of the solar cells. This finding underscores the importance of optimizing the layer thickness during the fabrication

process to achieve higher efficiencies in solar cell design.

Furthermore, the provided maximum achievable photovoltaic (PV) parameters offer additional valuable information. The reported fill factor (FF) of 89.06% indicates that the solar cells are capable of efficiently utilizing the available power from the incident light. A high FF is desirable as it reflects the ability of the solar cells to minimize losses and maximize power output.

The short-circuit current density (JSC) value of 35 mA/cm^2 is also significant. It signifies the current generated when the solar cells are under short-circuit conditions, indicating their capacity to produce a substantial amount of current. This characteristic is advantageous for applications where high current output is required, such as in power-hungry devices or systems.

Lastly, the open circuit voltage (Voc) corresponds to the maximum voltage that can be achieved across the solar cell terminals when there is no external load. The reported value of 1.17 volts implies a decent voltage output and suggests that the material properties and device design facilitate the separation and collection of charge carriers effectively.

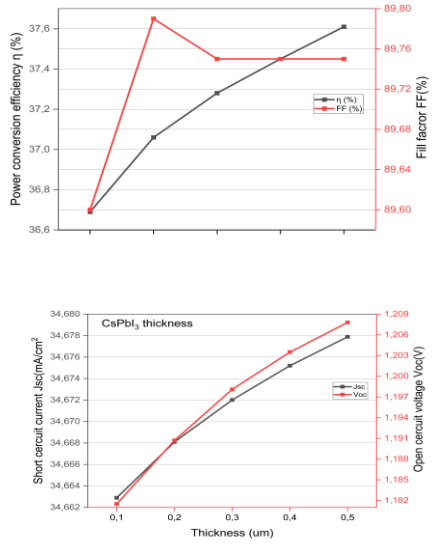

Fig 3 : The influence of $CsPbI_3$ thickness on the properties of solar cell.

In Fig 3, the relationship between the layer thickness of $CsPbI_3$ and the efficiency of a solar cell is demonstrated. The data presented in the figure shows that as the thickness of the $CsPbI_3$ layer increases, the efficiency of the solar cell exhibits a slight improvement, rising from 36.4% to 37.6%. Additionally, the figure provides information about the maximum achievable photovoltaic parameters, including the fill factor (FF), short-circuit current density (Jsc), and open-circuit voltage (Voc). The corresponding values for these parameters are reported as 89%, 34 mA/cm^2, and 1.2 V, respectively.

Efficiency Improvement: The small increase in efficiency from 36.4% to 37.6% indicates that there is a positive correlation between the thickness of the $CsPbI_3$ layer and the solar cell's performance. This suggests that increasing the layer thickness within the given range can lead to a marginal enhancement in the overall efficiency of the solar cell. However, it is worth noting that the improvement is relatively small, indicating that other factors might have a more substantial impact on the overall efficiency. Optimal $CsPbI_3$ Layer Thickness: The presented data does not provide information on the specific range of $CsPbI_3$ layer thicknesses tested or whether there is an optimal thickness for achieving maximum efficiency. Therefore, it is difficult to determine if the reported increase in efficiency from 36.4% to 36.5% represents the peak efficiency or if further thickness adjustments could yield even better results.

B. **Effect of Changing the absorber layer concentration of ($CsPbI_3$)**

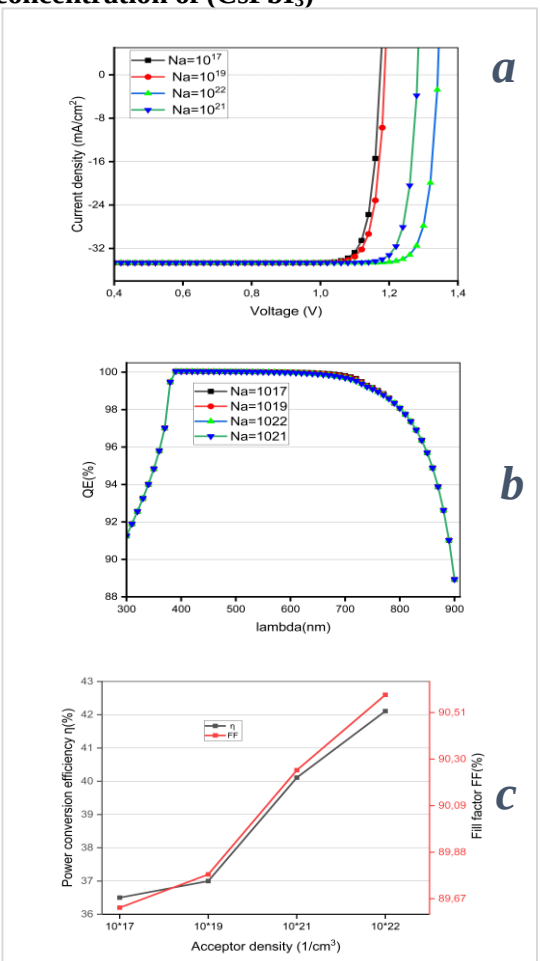

Fig 4: The influence acceptor density of $CsPbI_3$

In this analysis, we will examine the effect of acceptor density on the efficiency and other characteristics of a solar cell, as depicted in Figure 4 (a, b, c). The investigation focuses on the acceptor density range from 1×10^{17} cm^{-3} to 1×10^{22} cm^{-3} and its impact on efficiency (PCE), fill factor (FF), short-circuit current density (Jsc), voltage, and quantum efficiency.

Figure 4 (c) shows that increasing the acceptor density from 1×10^{17} cm^{-3} to 1×10^{22} cm^{-3} results in a considerable improvement in efficiency (PCE) and fill factor (FF). This indicates that higher acceptor densities lead to a more efficient solar cell design.

The impact of acceptor density on the J-V curves is illustrated in Figure 4 (a). Here, it can be observed that the current density (Jsc) remains stable at Jsc=-35.5 mA/cm^2, while the voltage increases as the acceptor density of the $CsPbI_3$ material increases. This indicates that increasing the acceptor density leads to higher voltages in the solar cell, which can positively influence the overall performance of the device.

Furthermore, the high quantum efficiency depicted in Figure 4 (b) highlights the efficient absorption of light in the visible range, contributing to the overall efficiency recorded, which reaches an impressive 42%.

C. Impact of Temperature on $CsPbI_3/CH_3NH_3SnBr_3$

Table 2: the effect of temperature changes on CsPbI3/CH3NH3SnBr3

Température(k)	Voc (V)	Jsc (mA/cm^2)	FF (%)	Ƞ (%)
270	1.2187	34.647355	90.62	38.26
290	1.1889	34.654433	90.04	37.10
310	1.1607	34.663072	89.20	35.89
340	1.1184	34.676344	88.13	34.18
370	1.0764	34.688851	86.89	32.44

Upon examining Table 2, it becomes apparent that as the temperature increases, the parameters of the solar cell exhibit a decline. Specifically, the efficiency of the solar cell decreases as the temperature rises. This finding suggests that higher temperatures have an adverse effect on the overall performance of the solar cell.

The observed reversal in the effect of temperature is an important finding, as it implies that higher temperatures have a detrimental impact on the performance of the solar cell. This effect can be attributed to several factors. For example, increased temperatures can lead to enhanced carrier recombination rates, which in turn reduces the efficiency of the solar cell. Additionally, higher temperatures may also affect the electrical properties and mobility of charge carriers, further impacting the performance of the solar cell.

These results highlight the significance of temperature control and management in photovoltaic systems. It underscores the need for appropriate cooling and thermal management strategies to maintain optimal operating conditions for solar cells, especially in environments with elevated temperatures.

D. Effects of Series Resistances on the performance of the Solar Cell

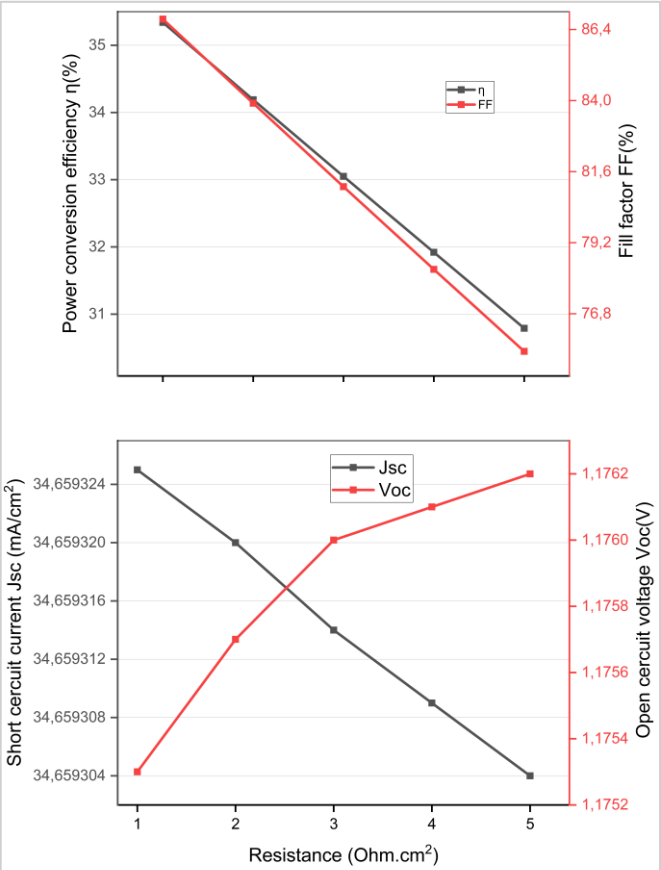

Fig 5: Effects of series resistance on photovoltaic parameters

The analysis highlights the relationship between series resistance (Rs) and the fill factor (FF) and short-circuit current density (Jsc) of solar cells, emphasizing the agreement with existing literature. The findings Figure 5 indicate that an increase in Rs has an adverse effect on FF, and when Rs is remarkably high, it slightly affects Jsc.The observed degradation of FF due to an increase in Rs aligns with previous studies, suggesting that higher series resistance leads to a reduction in FF. This relationship is crucial because FF represents the ability of the solar cell to effectively utilize the available power from the incident light. The

reported degradation of approximately 2.82% in FF with each 0.01 W increase in Rs is slightly higher than that of conventional silicon (Si) solar cells, which exhibit a decrease of approximately 2.5% per 0.01 W increase in Rs. This comparison highlights the significance of managing and minimizing series resistance to maintain high FF values in solar cell designs.

Furthermore, it is noteworthy that while FF degrades at a rate of 3.6% with each 0.01 W increase in Rs, the efficiency of the solar cells degrades at a much lower rate of only 1.14%. This finding indicates that the overall performance of the solar cells is relatively less affected by increases in Rs compared to FF. The efficiency of a solar cell reflects its ability to convert sunlight into usable electrical energy, and a lower degradation rate suggests that the impact of increased series resistance on the overall energy conversion is relatively minimal.

These observations provide encouraging insights into the behavior of solar cells in the presence of increased series resistance. While higher Rs negatively influences FF and has a slight impact on Jsc, the overall degradation in efficiency remains relatively low. This implies that even in the presence of increased series resistance, the solar cells can still maintain a considerable level of energy conversion efficiency.

IV. CONCLUSION

The study aimed to investigate the influence of various physical parameters on the performance of a $CsPbI_3$-based heterojunction solar cell. The parameters examined included temperature, acceptor density, i-$CH_3NH_3SnBr_3$ thickness, and $CsPbI_3$ absorber layer thickness, as well as the effect of series resistance.

To ensure accurate simulations, prior research and experimental findings were used to stabilize the Glass/ETL/$CH_3NH_3SnBr_3$/$CsPbI_3$/HTL parameters before proceeding with the device optimization process. This step helped establish a reliable baseline for the subsequent experiments.

After conducting the optimization, an interesting result was obtained, with an efficiency of 42% achieved using a $CsPbI_3$ thickness of 0.3 um, $CH_3NH_3SnBr_3$ thickness of 0.9 um, and acceptor density of 10^{22} cm^{-3}. This finding suggests that the performance of the $CsPbI_3$-based heterojunction solar cell is more favourable in lower temperature environments indicating the importance of controlling the operating temperature for optimal efficiency. Additionally, efficiency can be further enhanced by doping the $CsPbI_3$ layer with elements such as titanium or Tin. This doping approach can modify the properties of the absorber layer and improve the overall performance of the solar cell.

Additionally, the study revealed that the impact of increased series resistance on the overall energy conversion is relatively minimal. This finding suggests that the solar cell exhibits a lower degradation rate, meaning that the loss in efficiency due to increased series resistance is not significant compared to the gains achieved through other optimizations.

Overall, this study provides valuable insights into the influence of physical parameters on the performance of a $CsPbI_3$-based heterojunction solar cell and highlights potential strategies for further improving its efficiency. In summary, this research provides valuable insights into the optimization of $CsPbI_3$-based heterojunction solar cells, it can also future investigations can build upon these findings to explore additional parameters and techniques, further improving the design and functionality of $CsPbI_3$-based heterojunction solar cells.

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