**Conversion efficiency optimization of all-inorganic perovskite** $CsPbI\_{3-x}Br\_{x}$ **solar cell with** $Cu\_{2}O$ **and** $SnO\_{2}$ **as transport layers**

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ABSTRACT

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| --- |
| In this modelling study, carried out using SCAPS 1 D software, we optimized the conversion efficiency of our Al/$ SnO\_{2}/CsPbI\_{3-x}Br\_{x}$/$ Cu\_{2}O/ITO$ structure device. The study reveals that $CsPbI\_{3}$ is the best absorber material that can be obtained from $CsPbI\_{3-x}Br\_{x}$, by varying x between 0 and 3 (x ꞓ ℕ). The study shows that the suitable values for the thickness of the hole ($Cu\_{2}O)$ and electron ($SnO\_{2})$ transport layers are 1000 nm and 30 nm respectively. For the $CsPbI\_{3}$ absorber of the solar cell, a thickness of 1000 nm and a defect density of $10^{10}$ $cm^{-3}$ are required to give a conversion efficiency of 20.43% to the device. Fixing the ITO back contact energy at 4.7 eV leads to an optimization of the conversion efficiency of the solar cell which can reach up to 26.76 % giving our device one of the best conversion efficiencies. |

***Keywords:***modelling, $CsPbI\_{3-x}Br\_{x}$, absorber, $CsPbI\_{3}$ material and conversion efficiency (PCE).

1. INTRODUCTION

The conversion efficiencies of perovskite-based solar cells are increasing steadily and are expected to reach around 25.7% [2] by 2022. It is true that perovskite cells are experiencing a boom in efficiency, especially organic-inorganic hybrid perovskites. The latter suffer from a crucial problem of instability, moisture degradation and thermal environment [3], which remains a serious challenge for their commercial application. To overcome these shortcomings, all-inorganic perovskites based on $CsPbI\_{3-x}Br\_{x}$, have attracted a lot of attention as a light absorbing layer material due to its absorptive capacity, excellent thermal stability and suitable photo-physical properties [3]. As a result, the yields of all-inorganic perovskites have evolved significantly, but still remain below their hybrid counterparts. The efficiency of all-inorganic PCS is 60 % of the theoretical efficiency [11]. In order to improve the conversion efficiency of all-inorganic photovoltaic cells, the choice of transport layers is very important, because when a beam of light reaches the cell, the perovskite absorber material in the cell generates electron-hole pairs first. Then the transport layers will extract the carriers from the active layer and transport them to the bilateral electrodes respectively [11]. The choice of the thickness and defect density of the absorber will also be crucial in improving the conversion efficiency of the perovskite-based solar cell [10].

In this study, we set the electron ($SnO\_{2})$ and hole ($Cu\_{2}O)$ transport layers which are the best ETL/HTL combination [1], we will first study the best absorber obtained from perovskite $CsPbI\_{3-x}Br\_{x} $by varying x between 0 and 3 (x ꞓ ℕ). Next, we will choose the best material obtained study the effect of its thickness. Also study the effect of the thickness of the interface layers (HTL, ETL). We will study the effect of the defect density of the absorbing layer. Finally, we will evaluate the effect of the ITO back contact on the conversion efficiency of the solar cell.

**Methodology:**

**2.** **Modelling Structure**

In this study, we will model the (n-i-p) structure of Al/$ SnO\_{2}/CsPbI\_{3-x}Br\_{x}$/$ Cu\_{2}O/ITO$ configuration which is shown in Figure 1. In our absorber layer, we will vary x between 0 and 3 with (x ꞓ ℕ). The variation of x leads to different types of materials which are: $CsPbI\_{3}, CsPbI\_{2}Br, CsPbIBr\_{2} and CsPbBr\_{3}$. The simulation parameters are obtained using the solution of the fish equation (1) and the continuity equation for each electron and hole (2) and (3). Solving these equations also allows the calculation of the short-circuit density ($J\_{sc}$), quantum efficiency (QE), voltage ($V\_{oc}$), filling factor (FF) (4) and conversion efficiency (PCE) (5). The modelling is carried out using the SCAPS 1 D software [12, 14] in the standard AM 1.5 G spectrum (100 W/$m^{2}$, T= 300 K) and the parameters used for the different layers are taken from the literature**.**







n is the free electrons and p is the free holes, $n\_{t}$ and $p\_{t}$ are the trapped electrons and holes $N\_{D}^{+}, N\_{A}^{-}$ the ionized donor and acceptor doping concentrations respectively.





* FF= form factor
* $V\_{max}$= maximum voltage
* $J\_{max}$= maximum current density
* $V\_{oc}$= open circuit voltage
* $J\_{sc}$= = short circuit current density
* $P\_{in}$= incident power
* PCE= conversion efficiency



**Fig. 1. Model of the studied cell device**

 **Table 1. Cell structure modelling parameters**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | $$Cu\_{2}O$$$[$1,12,14] | $$CsPbI\_{3}$$[12,16] | $$CsPbI\_{2}Br$$[4,5,16, 17] | $$CsPbIBr\_{2}$$[6,7,16,18] | $$CsPbBr\_{3}$$[13,15,16,19] | $$SnO\_{2}$$[1,8,12] |
| $N\_{A}$($cm^{-3}$) | $$10^{18}$$ | - | - | - | - | - |
| $N\_{D}$($cm^{-3}$) | - | $$10^{15}$$ | $$10^{15}$$ | $$10^{15}$$ | $$10^{15}$$ | $$10^{15}$$ |
| $$ℇ\_{r}$$ | 7.1 | 6 | 8.6 | 8 | 6.5 | 9 |
| Χ (eV) | 3.2 | 3.95 | 3.8 | 3.6 | 3.95 | 4 |
| $E\_{g}$(eV) | 2.17 | 1.73 | 1.82 | 2.05 | 2.3 | 3.5 |
| $µ\_{n}$($\frac{cm^{2}}{V}$/s) | 200 | 16 | 200 | 20 | 25 | 20 |
| $µ\_{p}$($\frac{cm^{2}}{V}$/s) | 80 | 16 | 200 | 20 | 25 | 10 |
| $N\_{t}$($cm^{-3}$) | $$10^{15}$$ | 2.67$10^{14}$ | 3.64$10^{15}$ | $$10^{15}$$ | 1.5$10^{12}$ | $$10^{15}$$ |
| $N\_{C}$($cm^{-3}$) | $$2.210^{18}$$ | 1.1$10^{20}$ | 2.2$10^{18}$ | 2$10^{18}$ | 4.94$10^{17}$ | 4.36$10^{18}$ |
| $N\_{V}$($cm^{-3})$ | $$1.810^{19}$$ | 8$10^{19}$ | 1.8$10^{19}$ | 5$10^{18}$ | 8.47$10^{18}$ | $$2.610^{21}$$ |
| Thickness (nm) | 80 | 490 | 490 | 490 | 490 | 70 |

In the table above, $N\_{C}$ and $N\_{V}$ are the effective conduction band and valence band densities, $N\_{A} $and $N\_{D}$ are the acceptor and donor densities, $µ\_{p} $and $µ\_{n}$ are the hole and electron mobility, $N\_{t}$ is the defect density, χ is the electron affinity and $ℇ\_{r}$ is the relative permittivity.

3. results and discussion

3.1 Determination of the best absorber material

In this section, we will investigate the yields of different types of materials obtained from the $CsPbI\_{3-x}Br\_{x}$ absorber by varying x (0≤x≤3, x ꞓ ℕ) based on the Al/$ SnO\_{2}/CsPbI\_{3-x}Br\_{x}$ /$Cu\_{2}O/ITO$ structure. The simulation results obtained from the data in Table 1, are shown in Figures 2, 3 and 4. Figure 2 illustrating the current density (J) versus open circuit voltage ($V\_{oc})$ shows that the current density value obtained with the $CsPbI\_{3}$ material is better compared to its other counterparts ($CsPbI\_{2}Br,CsPbIBr\_{2}$ and $CsPbBr\_{3})$ as can be seen from Table 2. This can be explained by the fact that the charge carrier displacement in the $CsPbI\_{3}$ material is easier than in the other materials, thus facilitating a diffusion of electrons to the outer layers resulting in the increase of the current density. Furthermore, we notice in Figure 2 that the open circuit voltage ($V\_{oc})$ of $CsPbI\_{3}$ is smaller than those of other materials. Since the value of the gap energy conditions the open-circuit voltage across the barrier height of the junction, Figure 3 effectively shows that the materials ($CsPbI\_{2}Br,CsPbIBr\_{2}$ and $CsPbBr\_{3})$ have a much higher gap energy than $CsPbI\_{3}$, which translates into their large open-circuit voltage value ($V\_{oc})$, hence their low current density compared to that of the $CsPbI\_{3}$ material. Figure 4 showing the quantum efficiency of the different materials confirms that the $CsPbI\_{3}$ material has the largest spectral response width, thus proving that the $CsPbI\_{3}$ material has the largest optical absorption capacity than the other materials ($CsPbI\_{2}Br,CsPbIBr\_{2}$ and $CsPbBr\_{3})$ hence these better conversion performances, as it is translated in Table 2. Therefore, in the further work, we will use the $CsPbI\_{3}$ material as an absorber layer and perform studies on parameters that can improve the conversion efficiency of our photovoltaic cell.



**Fig. 2. Characteristics (J-V) of different materials obtained from the** $CsPbI\_{3-x}Br\_{x}$ **absorber.**



**Fig. 3. Alignment of the energy levels of the different layers of the device**

**Table 2. Performance of different materials obtained from the** $CsPbI\_{3-x}Br\_{x}$ **absorber.**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | $V\_{oc}$ (V) | $$J\_{sc}\left({mA}/{Cm^{2}}\right)$$ | FF(%) | PCE(%) |
| $$CsPbI\_{3}$$ | 1.18 | 18.51 | 86.41 | 18.86 |
| $$CsPbI\_{2}Br$$ | 1.28 | 16.34 | 84.26 | 17.67 |
| $$CsPbIBr\_{2}$$ | 1.51 | 11.21 | 73.76 | 12.48 |
| $$CsPbBr\_{3}$$ | 1.65 | 7.74 | 76.10 | 9.75 |



**Fig. 4. Quantum efficiency (QE) of different materials obtained from perovskite** $CsPbI\_{3-x}Br\_{x}$**.**

3.2 Effect of the thickness of the $CsPbI\_{3}$

In this section we will try to optimize the performance of the solar cell by varying the thickness of the $CsPbI\_{3}$ absorber between 100 nm and 1000 nm. The $CsPbI\_{3}$ absorber material plays a very important role in the performance of the solar cell as it is the material that absorbs the light and subsequently generates electron-hole pairs. The results of modelling the thickness of the $CsPbI\_{3}$ material are shown in Figures 5 and 6. Figure 5 shows that as the thickness of the absorber is increased, the current density increases and becomes saturated at 800 nm. The same is true for the value of the photovoltaic parameters ($J\_{sc}$ and PCE) which increases with thickness as shown in figure 6. However, Figure 6 shows a rapid decrease in the voltage ($V\_{oc}$) and form factor (FF) of the cell with increasing absorber thickness. This can be explained by the fact that increasing the thickness of the absorber causes the series resistance to rise, thus decreasing the form factor (FF). On the other hand, the decrease in open circuit voltage ($V\_{oc}$) is due to the fact that there is an interdependence between the voltage and the form factor. Figure 6 also shows that the best conversion efficiency value of the cell is 20.08% for a thickness of 1000 nm. It can be deduced that a larger absorber thickness encourages a greater creation of electron-hole pairs and avoids recombination, thus increasing the efficiency. For the rest of our study, we will work with the optimal value of 1000 nm for the $CsPbI\_{3}$ material layer.



**Fig. 5. Characteristic (J-V) thickness of the** $CsPbI\_{3}$ **material.**

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**Fig. 6. Photovoltaic parameters of the** $CsPbI\_{3}$ **material:** $V\_{oc}$ **(a),** $J\_{sc}$ **(b), FF(c) and PCE (d).**

**3.3 Effect of the thickness of the hole transport layer (HTL)**

In this work, we used the $Cu\_{2}O$ layer as the hole transport layer and its thickness value is varied between 100 nm and 1000 nm. Figure 7 illustrating the electrical parameters of this layer shows an ascending trend for the open-circuit voltage ($V\_{oc}$) (a), current density (b) and conversion efficiency (d). On the other hand, with regard to its form factor (c), we note a rapid decrease in its value as a function of the increase in the thickness of the layer. The stimulated cell shows that increasing the thickness of the hole transport layer $Cu\_{2}O$ improves the conversion efficiency of the device from 18.88 % for a thickness of 100 nm to 19.10 % for 1000 nm. This can be explained by the fact that the $Cu\_{2}O$ layer is located at the back of the absorber layer so a large thickness allows it to reduce recombination and to be able to transport the carriers created to the back contact hence the good optical efficiency obtained with a thickness of 1000 nm.

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**Fig. 7. Electrical parameters of the HTL layer (**$Cu\_{2}O$**):** $V\_{oc}$ **(a),** $J\_{sc}$ **(b), FF(c) and PCE (d).**

**3.4 Effect of the thickness of the ETL layer (**$SnO\_{2}$**)**

In this section, we have varied the thickness of the ETL layer ($SnO\_{2}$) between 10 nm and 60 nm. Figure 8 shows that varying the thickness of the electron transport layer ($SnO\_{2}$) from 10 nm to 30 nm causes an exponential increase in the parameters of open circuit voltage (a), current density (b), form factor (c) and conversion efficiency (d) and reaches their maximum value which is 1.18 V, 18.52$ {mA}/{cm^{2}}$, 86.44 % and 18.89 % for a thickness of 30 nm respectively. Beyond this value, the increase in $SnO\_{2}$ thickness has no effect on the $V\_{oc}$ and FF of the cell. On the other hand, we note a drastic drop in $J\_{sc}$ and PCE when we continue to increase the thickness of the $SnO\_{2}$ layer. The explanation is simple in that the electron transport layer ($SnO\_{2}$) is located in front of the absorber layer $CsPbI\_{3}$, so increasing its thickness causes an increase in series resistance, which impairs the transfer of the photo-carriers to the back layers, hence the decrease in conversion efficiency of our device. Therefore, we will optimize the device efficiency by using $SnO\_{2}$ as the ETL layer by taking its best thickness which is 30 nm.

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|  |  |

**Fig. 8. Electrical parameters of the ETL layer (**$SnO\_{2}$**):** $V\_{oc}$ **(a),** $J\_{sc}$ **(b), FF (c) and PCE (d).**

**3.5 Optimizing the conversion efficiency of the device**

In this section, we will try to optimize the performance of our $CsPbI\_{3}$ based cell device with a thickness of 1000 nm, using the HTL layer ($Cu\_{2}O$) for a thickness of 1000 nm and the ETL layer ($SnO\_{2}$) of 30 nm thickness. Figure 9 translates the J-V (9 a) and QE (9 b) characteristics obtained from our device with these new thickness values. The modelling results show a clear improvement in the photovoltaic parameters of the cell with a PCE of 19.89%, a $J\_{sc}$ current density of 20.48 ${mA}/{cm^{2}}$, a form factor of 84.95 % and an open circuit voltage of 1.14 V. We also note an improvement in the width of the absorption spectrum (Figure 9 b) of our device, which reaches its maximum peak at 400 nm and remains almost constant until 650 nm. This gives our cell good absorption in the visible range. This improvement of the parameters is partly due to the choice of the ideal thicknesses of the different layers constituting the device, thus facilitating the reduction of the series resistance and an increase in the shunt resistance leading to a good displacement of the electron-hole pairs, hence the efficiency obtained. The conversion efficiency can be further improved if we can mitigate the traps in the $CsPbI\_{3}$ absorber layer.





**Fig. 9. Characteristics of the optimized device: J-V (a) and QE (b)**

**3.6 Effect of the defect density (**$N\_{t}$**) of the** $CsPbI\_{3}$ **absorber layer on cell performance**

To explain the poor performance of all-inorganic perovskite solar devices, we will study here the defects in the $CsPbI\_{3}$ absorber layer of the cell. The results obtained in figures 10 and 11 reflect the influence of the defect density ($N\_{t}$) of the $CsPbI\_{3}$ absorber layer on the photovoltaic properties. According to Figure 10 for defect values ($N\_{t}\leq 10^{14}$ $cm^{-3}$), the current density (J-V) is at its best value (10 a) and the cell shows a good spectral response (10 b). Beyond $10^{14}$ $cm^{-3}$, the injection of impurity into the $CsPbI\_{3}$ absorber layer, leads to a drastic drop in the current density and weakens the absorption capacity of the cell, which causes the conversion efficiency to drop from 20. 43 % for $N\_{t}=10^{10}$ $cm^{-3}$ to 0.25 % for $N\_{t}=10^{18}cm^{-3}$. The remark is the same, weak defects ($N\_{t}\leq 10^{14}$ $cm^{-3}$) have no effect on the electrical properties of the cell ( $V\_{oc}$, $J\_{sc}$, FF et PCE) (Fig. 11). When the impurities in the absorber layer $CsPbI\_{3}$ are higher than $10^{14}$ $cm^{-3}$, the value of the contact resistance increases, which leads to a filling factor (FF), open-circuit voltage ($V\_{oc}$), short-circuit current density ($J\_{sc}$) and conversion efficiency (PCE) at low $N\_{t}=10^{18}cm^{-3}$ as shown in Figure 11.





**Fig. 10. Characteristics of the** $CsPbI\_{3}$ **absorber as a function of the variation of the total defects: J-V (a) and QE (b).**



**Fig. 11. Electrical parameters of the** $CsPbI\_{3}$ **absorber as a function of total defect variation:** $V\_{oc}$ **(a),** $J\_{sc}$ **(b), FF (c) and PCE (d).**

**3.7 Effect of the ITO work function on the solar cell**

In this section, we study the influence of the work function of the ITO backside layer, whose energy is reported in the literature to be between 4.5 and 4.7 eV [9]. The work function of the back contact is a significant factor in achieving a reasonable integrated voltage in solar devices. To observe how the variation of the energy range of the ITO contact can have an impact on the $CsPbI\_{3}$ device, the modelling results are summarised in Figure 12 and Table 3. It can be clearly seen (Fig.12) that there is an overlap in the current density of the work function between 0 and 1.2 V. Above this value, there is a drop in the current density as a function of the energy value used for the ITO back layer. Table 3 shows that the performance of the solar cell increases linearly with the change in energy of the ITO contact. The conversion efficiency of the device increases from 20.43 % without back contact to 26.76 % with ITO for an energy of 4.7 eV, i.e. an increase of 76.3 %.

**Table 3**: Performance of the device as a function of the variation in the energy of the ITO back contact.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| ITO contact energy (eV) [9] | $V\_{oc}$ (V) | $$J\_{sc}\left({mA}/{Cm^{2}}\right)$$ | FF (%) | PCE (%) |
| 4.5 | 1.51 | 20.46 | 73.29 | 22.63 |
| 4.6 | 1.60 | 20.52 | 75.30 | 24.79 |
| 4.7 | 1.66 | 20.52 | 78.633 | 26.76 |

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**Fig.12. Characteristics (J-V) of the solar cell as a function of the variation of the ITO back contact energy.**

4. Conclusion

Using SCAPS 1 D software, modelling performed on our cell device based on the (n-i-p) configuration with Al/$ SnO\_{2}/CsPbI\_{3-x}Br\_{x}$/$ Cu\_{2}O/ITO$ structure revealed excellent performance. The study shows that the $CsPbI\_{3}$ material is the better absorber obtained from $CsPbI\_{3-x}Br\_{x}$ than its counterparts by varying x between 0 and 3 (x ꞓ ℕ). For the hole ($Cu\_{2}O$) and electron ($SnO\_{2}$) transport layers, the appropriate thicknesses are 1000 nm and 30 nm, respectively. Hence, for the $CsPbI\_{3}$ absorber of the solar cell, a thickness of 1000 nm and a defect density of $10^{10}$ $cm^{-3}$ are needed to give a conversion efficiency of 20.43% of the device. Fixing the energy of the ITO back contact at 4.7 eV leads to an increase in the conversion efficiency of the solar cell which can reach 26.76 % which gives our device one of the best conversion efficiencies. The practical implementation of this work can be a great advance in the field of all-inorganic perovskite solar cells.

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