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# Performance Optimization of MASnI3-based Perovskite Solar Cells

***Abstract***. *Solar cells of hybrid organic-inorganic perovskite have attracted researchers and scientists all over the world. Perovskite solar cells outperform conventional silicon solar cells by achieving higher conversion efficiency with a more stable performance. In this paper, a typical perovskite solar cell consists of 6 principal layers of materials: a protective glass layer, thin fluorine Doped Tin Oxide (FTO), $Cd_{0.5}$ $Zn_{0.5}S$ as electron transportation layer (ETM), $MASnI_3$ as perovskite active layer, CuSCN as hole transportation layer (HTM) and another gold (Au) electrode were utilized. This paper summarizes the work that centred on the selective use of composite materials of the perovskite solar cell with a variation of the perovskite layer thickness. An optimization procedure is applied to increase the conversion efficiency and enhance the overall performance by varying the thickness and doping concentration of the main cell layers (i.e. ETM, absorber and HTM). The results showed that, by employing the optimum parameters, the conversion efficiency was increased from 12.86 to 26.68%.*

***Streszczenie.*** *Ogniwa słoneczne z hybrydowego organiczno-nieorganicznego perowskitu przyciągają badaczy i naukowców na całym świecie. Ogniwa słoneczne Perovskite przewyższają konwencjonalne krzemowe ogniwa słoneczne, osiągając wyższą wydajność konwersji przy bardziej stabilnej wydajności. W tym artykule typowe perowskitowe ogniwo słoneczne składa się z 6 głównych warstw materiałów: ochronnej warstwy szklanej, cienkiej domieszkowanej fluorem tlenku cyny (FTO), Cd0,5 Zn0,5S jako warstwy transportu elektronów (ETM), MASnI3 jako warstwy aktywnej perowskitu , zastosowano CuSCN jako warstwę transportującą dziury (HTM) i inną złotą (Au) elektrodę. Ten artykuł podsumowuje prace, które koncentrowały się na selektywnym wykorzystaniu materiałów kompozytowych perowskitowego ogniwa słonecznego ze zmianą grubości warstwy perowskitu. Stosowana jest procedura optymalizacji w celu zwiększenia wydajności konwersji i poprawy ogólnej wydajności poprzez zmianę grubości i stężenia domieszkowania głównych warstw komórek (tj. ETM, absorbera i HTM). Wyniki wykazały, że przy zastosowaniu optymalnych parametrów wydajność konwersji wzrosła z 12,86 do 26,68%.* (***Optymalizacja wydajności ogniw słonecznych perowskitowych opartych na MASnI3***)

**Keywords:** Modelling, Simulation, Perovskite Solar Cell, Photovoltaics, Inorganic Materials, Organic Materials.
**Słowa kluczowe:** ognia fotowoltaiczne Perovskite, optymalizacja

## Introduction

The silicon solar cell has so far been successfully reached an efficiency of 12 to 17.5 %, resulting in a comprehensive search for modern, more effective content. Thus, scientists who are working on hybrid photovoltaic materials started to investigate their efficiency extensively. Photovoltaic hybrids have opened the door for a new era by achieving better performance compared to inorganic silicon solar cells. Silicon was the main material used for manufacturing solar cells since the 1950s. Organic and inorganic hybrids have gained great attention by introducing perovskite solar cells since 2009 with efficiency starting from 3.8% to more than 23.3%. Perovskite solar cells have shown an extremely low cost, low complexity, and high system efficiency combination [1]. The perovskite solar cell (PSC) does not only absorbs the visible light spectrum, but also the near-infrared radiation. In contrast, only the visible light spectrum can be absorbed by the silicones. Solar Cell Capacity Simulator (SCAPS) 1D was extensively used previously to analyze perovskite solar cells and investigate the different parameters that affect the conversion efficiency. Actual experimental data were in the perovskite solar cell to model the solar cell perovskite characteristics. It is also examined the effect on solar cell efficiency of absorber size, doping concentration, and defects [1, 2].

Any substance with a similar crystal structure in a different transition state to the mineral is referred to as perovskite. $ABX_3$ reflects the crystal structure of perovskite in which A is a large organic or inorganic cation, B is a tinier inorganic cation such as ($Cu_2$ +, $Sn_2$ +, $Pb_2$ +, etc.) [3], and $X_3$ is a halogen ion Cl-, Br- and I-) which is capable of interacting with both cation(s) A and B. There is a straight bandgap of two the Perovskites, giving it the requisite optical characteristics for harvesting near-infrared (NIR) and ultraviolet (UV) light and can then be exploited by the perovskites active layer [4-5]. The PCE of the perovskite solar cell is rising very rapidly. The perovskite makes a promising candidate in this comparison. The main aim of the design of a highly efficient solar cell is to maximize the effective energy conversion (PCE) ratio to cost. And due to this rapid investigation and enhancement of the perovskite band, around 2013-2018, an efficiency of 15.7% to 22.7% were reported in the literature [6-7].

Among various perovskite materials such as $MAPbBr_3$, $MAPbCl_3$, $MAPbBr_3$, $MASnI_3$ and $MAPbI_3$, it is observed that $MASnI_3$ iodide is a good candidate due to its excellent electrical and optical properties, low-temperature solvability, long-life, and ferroelectricity. With various design techniques not only for the absorber layer but also in all other six layers, the efficiency of perovskite solar cells can be further enhanced [8-9].

In this paper, a parametric study is performed on the planar perovskite solar cells with a structure of FTO/ $Cd_{0.5}Zn_{0.5}S$/ $MASnI_3$/CuSCN to find the optimum layer thickness and doping concentration to increase the overall conversion efficiency.

## Cell structure and input parameters

The structure of the proposed cell in the present work is based on a perovskite solar cell. As shown in figure (1), the structure consists of four layers, $Cd_{0.5}$ $Zn_{0.5}$ S as ETL layer, $MASnI_3$ as the absorber layer, CuSCN as HTL layer, and fluorine-doped tin oxide (FTO) as the transparent conducting oxide. The input parameters of the reference cell were taken from literature [10], and are listed in table 1. The structure was studied under the STC which is at a room temperature of 300 K, and 1000 W/m$^2$ irradiance levels.

The performance parameters of the reference cell, which are represented by JSC, VOC, FF, and efficiency, are calculated based on the basic parameters of the materials. The major parameters that have a direct impact on the cell performance are the doping density, the thickness, and the defect density of the layers. SCAPS simulation software is employed to perform all the necessary calculations [10].

Table 1. Input parameters of the reference cell taken from Ref. [10].

| Parameters | FTO | $Cd_{0.5}Zn_{0.5}S$ | $MASnI_3$ | CuSCN |
|---|---|---|---|---|
| Thickness (μm) | 0.2 | 0.2 | 0.2 | 0.2 |
| Eg (eV) | 3.5 | 2.8 | 1.3 | 3.4 |
| χ (eV) | 4 | 3.8 | 4.17 | 1.9 |
| εr | 9 | 10 | 8.2 | 10 |
| $N_C$ ($cm^{-3}$) | $10^{19}$ | $10^{18}$ | $10^{18}$ | $1.7 \times 10^{19}$ |
| $N_V$ ($cm^{-3}$) | $10^{19}$ | $10^{18}$ | $10^{18}$ | $2.5 \times 10^{21}$ |
| $\mu_n$ (cm2/Vs) | 100 | 100 | 1.6 | 0.0001 |
| $\mu_p$ (cm2/Vs) | 25 | 25 | 1.6 | 0.1 |
| $N_d$ ($cm^{-3}$) | $10^{15}$ | $10^{15}$ | 0 | 0 |
| $N_a$ ($cm^{-3}$) | 0 | 0 | $10^{15}$ | $10^{15}$ |
| $N_t$ ($cm^{-3}$) | $10^{14}$ | $10^{14}$ | $10^{14}$ | $10^{14}$ |

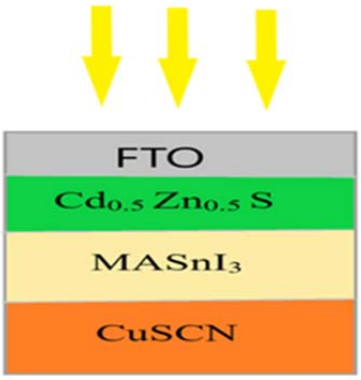


Fig. 1. Solar cell structure.

**Parametric study**

**a. CuSCn layer:**

The first step of the parametric study is to estimate the effect of the doping, the thickness, and the defect density variation in this layer on the performance of the cell. The simulation has been carried out by changing the doping density in this layer $N_a$ from $10^{15}$ to $10^{19}$ $cm^{-3}$. It is obvious from the results shown in figure (2) that increasing the carrier concentration in this layer has a significant impact on the whole performance of the cell, an increase in HTL acceptor doping concentration will reduce the resistivity of the HTL and therefore will enhance the current in the solar cell, which will cause the PCE to increase [10]. A slight increase was observed in the $J_{SC}$ from 23.846 to 25.044 $mA.cm^{-2}$ while the $V_{OC}$ was increased from 0.433 to 0.705 V, and thus the FF increased and consequently the efficiency of the cell was increased dramatically from 6.39 to 12.86 % with doping density. On the other hand, it was found that changing this layer thickness from 0.2 to 1 μm in a step of 0.2 does not affect the cell performance, and the short circuit current, as well as the open-circuit voltage, were constant at 25.044 $mA/cm^2$ and 0.705 V respectively, while the power conversion efficiency was kept at 12.86 %.

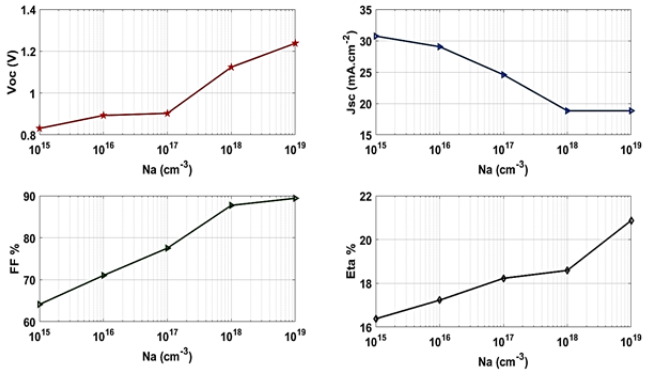


Fig. 3. The impact of Na variation in the MaSnI3 layer on the cell parameters.

b. **MASnI3 layer**

On the other hand, the curves in figure (4) show a similar trend, as the absorber layer thickness increases, the $V_{OC}$, $J_{SC}$, and PCE elevate while the FF was decreasing from 75.56 to 64.13 %. The increment in the $J_{SC}$ was due to the high absorption of photons by this layer [10]. As a result, the elevation of the excess carrier concentration causes the $J_{SC}$ to increase and consequently the efficiency.

The optimum values of the doping density, as well as the thickness for this layer, are $10^{19}cm^{-3}$ and 1 μm, respectively, which leads to a maximum PCE of more than 20 %.

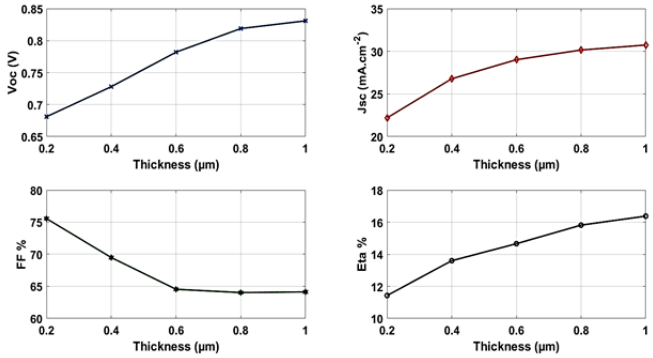


Fig. 4. The impact of the MaSnI3 layer thickness on the cell parameters.

The defect density variation has no noticeable influence in this layer, as $N_t$ changing from $10^{14}$ to $10^{17}$ $cm^{-3}$ there is no change in the output parameters of the cell and the efficiency was constant at 20.87 %.

**c. Cd0.5 Zn0.5 S layer:**

After having the optimum values of the thickness and doping density in the previous layer, the next step is to study the impact of the input parameters variation in this layer on the cell performance.

The thickness of this layer has a significant effect on the performance, as the thickness increases from 0.2 to 1 μm, the open-circuit voltage is almost constant at 1.2 V while the short circuit current elevates excessively from 5.308 to 22.658 $mA/cm^2$ and this is because thick layer in restricted range leads to higher absorption, and thus higher photo-generated carriers and higher $J_{SC}$, which finally leads to an increment in the efficiency [12] [13]. Figure (5) shows the aforementioned impact of layer thickness.

Increasing the doping density $N_d$ has a trivial impact on the performance of the cell, where the $V_{OC}$, as well as the PCE, starts to degrade gradually while the $J_{SC}$ increases slightly due to the increment in the carrier concentration. Thus, the optimum $N_d$ for this layer is $10^{15}$ $cm^{-3}$ that gives the highest PCE.

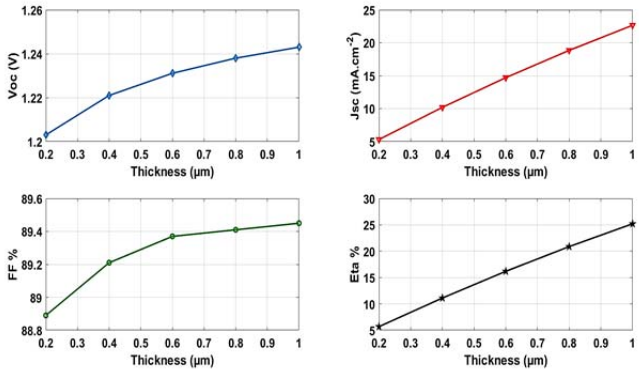


Fig. 5. The impact of this layer thickness on the output parameters.

**d. D.TO layer:**

Any solar cell with good design and high performance must have a thin layer of anti-reflection material of a heavily doped n-type material, which is in this work a layer of FTO. This layer will be a window for the light and acts as an anti-reflecting layer, which reduces the reflection losses at the same time; and this is the reason behind the advantage of using TCO material in any design. The effect of the doping and the thickness of this layer can be neglected as it will not contribute to the absorption and as a consequence in the generation of charge carriers.

**Optimum cell parameters**

The perovskite solar cell that has the best performance in this work is a cell that gives a PCE of 26.68 %, open-circuit voltage of 1.628 V, short circuit current of 22.682 mA/cm$^2$, and fill factor of 72.21 %. It has input parameters for the thickness and doping density as illustrated in table 2.

The energy band structure, as well as the quantum efficiency response of the optimum cell, are shown in figures (6) and (7).

Table 2. Input parameters of the optimum structure.

| Layer | Doping density (cm$^{-3}$) | Thickness (μm) |
|---|---|---|
| CuSCN | $10^{19}$ | 0.2 |
| $MASnI_3$ | $10^{19}$ | 1 |
| $Cd_{0.5}Zn_{0.5}S$ | $10^{15}$ | 1 |
| FTO | $10^{19}$ | 1 |

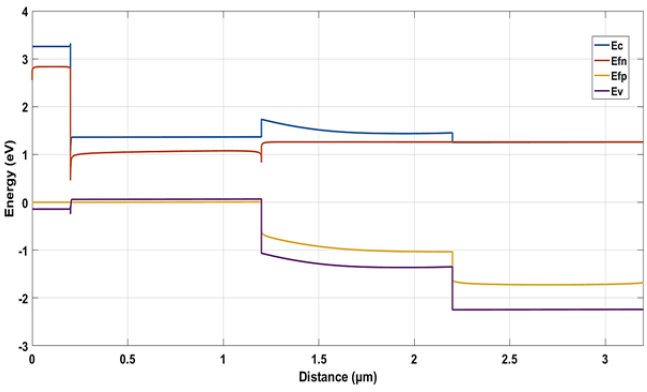


Figure. 6. Energy Band Structure of the optimum cell.

It can be observed from the band diagram of the perovskite layers (figure (6)) that the majority of photogenerated carriers are produced at the interface layers (HTM/Absorber and Absorber/ETM), thus, it is quite necessary to have these interfaces optimized and aligned properly in order to increase the open circuit voltage and hence the conversion efficiency. It is also noticed that the due to the high band gap energy of the HTM layer, the valance band offset is increased, which results in an inefficient charge transport. The energy diagram of the perovskite solar cell should be investigated properly in order to have a clear understanding of the most important parameters that affect the cell's performance.

On the other hand, figure (7) clearly shows that the proposed perovskite cell exhibits a constant quantum efficiency over a wide range of wavelengths.

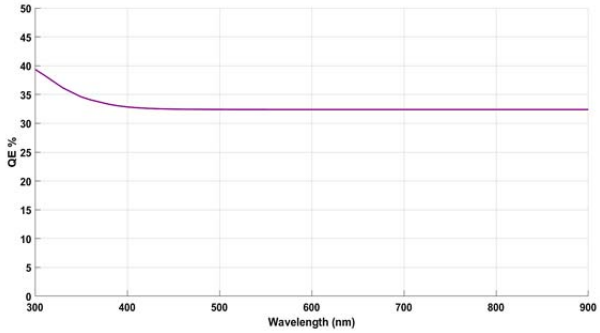


Fig. 7. The QE response with the wavelength.

**Conclusion**

In this paper, an optimization procedure has been applied to the planar perovskite solar cell that has the structure of FTO/ $Cd_{0.5}Zn_{0.5}S$/ $MASnI_3$/CuSCN to improve the overall conversion efficiency. SCAPS-1D simulator has been employed to calculate the cell's characteristics such as $V_{OC}$, $J_{SC}$, FF and efficiency as well as plotting the J-V characteristics. Throughout the parametric study of this work, the effect of thickness and doping concentration on the perovskite cell performance has been investigated for all layers. The results showed that increasing the thickness and the doping concentration of the absorber layer plays a significant role in increasing the total efficiency. It also found that the optimum thickness of the $Cd_{0.5}Zn_{0.5}S$ and $MASnI_3$ was 1μm, whereas it was 0.2 μm for the CuSCN layer. On the other hand, it was observed by simulation results that the optimum doping concentration is $10^{19}$ cm$^{-3}$ for the $MASnI_3$ and CuSCN layers, but it is $10^{15}$ cm$^{-3}$ for the $Cd_{0.5}Zn_{0.5}S$. Results demonstrate the promising future of perovskite solar cells by carefully tuning the most sensitive parameters that paly a significant role in the overall performance of the cell such as the layer thickness and the doping concentration as proposed in this paper. More parameters can be explored in future works and their impact on the cell's conversion efficiency can be investigated.

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