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# High Efficiency (22.46) of Solar Cells Based on Perovskites

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***Abstract*— In this research we have considered ($CH_3NH_3PbX_3$) (X=I,Cl,Br) as an absorber layer and Cu2O/spiro-OMeTAD/ P3hT/PEDOT:PSS as (HTM) along with PCBM/$TiO_2$ as (ETM). It is a solid-state planar heterojunction p-i-n solar cell with low p-type-doped; $CH_3NH_3PbX_3$ sandwiched between the p-type is called HTM layer and n-type. SCAPS-1D simulation software is used for numerical simulation to examine the influence of various electrical factors on the efficiency PCBM/$CH_3NH_3PbCl3$/P3hT,PCBM /$CH_3NH_3PbI_3$/P3hT,PCBM/$MAPbCl_3$/Cu2O,TiO2/$MAPbCl_3$/Sipro-OMeTAD, $TiO_2$/MAPbI3/Sipro-OMeTAD, PCBM /$CH_3NH_3PbBr3$/ PEDOT:PSS, and PCBM /$CH_3NH_3PbI_3$/ PEDOT:PSS heterojunction-based perovskite solar cell structures .With these variables an efficiency of 22.46% was obtained at 263.15(k). By using SCAPS simulation software**

***Keywords*—(Perovskite, efficiency, SCAPS-1D, Density of State, Fill Factor (FF))**

## I. INTRODUCTION

Photovoltaic (PV) devices convert solar radiation into power which is optimistic candidates to counterbalance carbon releases throughout providing a substitute way to meet up increasing require in energy utilization purity - crystalline silicon has achieved efficiencies (PCEs) above 26% [1] and long-term stability, making it an ideal manufactured goods for the promoter. However, emerging PV technologies based on thin films (<1 μm). There are fantastic technique of thin film of solar cells which was promising established ones such as Si, CdTe, and GaAs [2,3]. Lead halide perovskite solar cells (PSCs) have selected as one such proposed. In a few years, PSCs have produced PCEs parallel to those of traditional CdTe solar cells, reached to the 22% in 2016 [4]. Despite the high efficiencies, PSCs face challenges such as long-term durability that prevent them from competing with established technologies such as silicon solar cells in market Energy.. However, advancements in materials processing during the past 2 years have yielded remarkable progress in long-term material and device stability, enabling the research community to better recognize versus extrinsic degradation mechanisms, some of which are summarized here. Despite the rapid improvement in performance, there is wide space for reducing charge carrier recombination, both in the perovskites and at the interfaces within the device, to increase PCEs. Major challenges to long-term stability also remain.

Due to its utilizes of built-up, low cost of fabricate, excellent light-harvesting properties, and comparatively high performance, organic-inorganic hybrid perovskite solar cells have reached a lot of attention in the photovoltaic research community in recent years. This makes it more superior to other current solar cell materials. Lead-based perovskites ($CH_3NH_3PbX_3$, X= Cl, I, Br) Solar cells recently achieved a high efficiency more than 22%, far exceeding the efficiency of most thin film and organic solar cells. The poisonous presence of lead (Pb) poses a challenge for the commercialization availability of $MAPbX_3$. So, numerical analysis will play a key role in dealing with these solar cell issues because numerical analysis allows for versatility in the design of practical problems and simple experiment with various hypotheses. Sometimes, a complete collection of device characteristics can be quickly produced with just short time and effort. As a result, numerical analysis was used to resume the design parameters of solar cells as well as the impact of solar cell physical parameters on solar cell efficiency. Solar cell numerical analysis is carried out using a variety of simulation applications.


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Used the softwere the Solar cell capacitance simulator (SCAPS) program in this study; it is free and widely used in the research community. A numerical guide was suggested to improve the PCE of an experimentally developed solar cell in order to achieve successful design for powerful solar cells. According to the findings, the thickness of the absorber layer and interface defects have a significant impact on the PCE of a solar cell. Three primary layers sandwich the two conducting electrodes in perovskite-based solar cell. (The standard design of perovskite-based solar cell is as follows: Back electrode/ Hole Transport Material (HTM)/ Perovskite absorber / Electron Transport Material (ETM) / transparent electrode). In perovskite-based solar cells, electron-transport materials are also important. The results of a simulation analysis using the Solar Cell Capacitance Simulator as a simulation tool based on the position of the various components of the solar cell are discussed.

## II. Operation Theory

SCAPS-1D's core idea is to solve the equations of Poisson and continuity. Fig (1) illustrates the SCAPS-1D job technique. Any equation starts at the start of this period and uses the initial presumption that the quasi-Fermi level is used to achieve a balance. No lighting and voltage are added in this case [4].

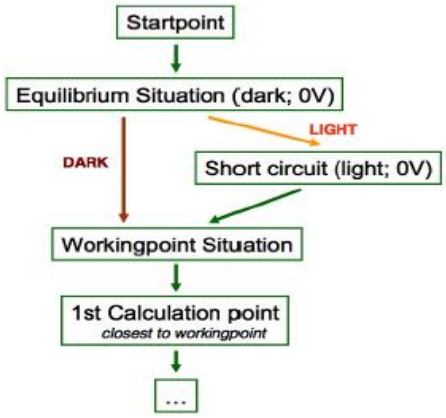


Fig.(1) SCAPS-1D's Operational Strategy [4]

SCAPS performs numerical calculations using the convergence of the Gummel type iteration approach and the Newton-Raphson algorithm. After choosing a calculation point, SCAPS will do iterative computations using the Newton-Raphson method until the ideal result is attained.
The key principle of the SCAPS-1D is to solve the Poisson equation for electrodes and holes and continuity equation [3].

$$\frac{\partial^2}{\partial x^2}\varphi(x) = \frac{q}{\varepsilon}[n(x) - p(x) - N_D^+(x) + N_A^-(x) - p_t(x) + n_t(x)] \quad (1)$$

$$q\frac{\partial n}{\partial t} = \frac{\partial J_n}{\partial x} + qG - qR$$
$$q\frac{\partial p}{\partial t} = -\frac{\partial J_p}{\partial x} + qG - qR \quad (2)$$

$$J_n = qn\mu_n\frac{\partial \varphi}{\partial x} + qD_n\frac{\partial n}{\partial x}$$
$$J_p = -qp\mu_p\frac{\partial \varphi}{\partial x} + qD_p\frac{\partial p}{\partial x} \quad (3)$$

where, $q$ is the elementary charge
$\varphi$ is the potential, $\varepsilon$ is the permittivity
$n$ is the density of free electron, $p$ is the density of free hole
$N_D^+$ is the ionised donor-like doping density
$N_A^-$ is the ionized acceptor-like doping density
$p_t$ is the trapped hole density
$n_t$ is the trapped electron density
$G$ is the optical generation rate
$R$ is the recombination rate
$D_n$ is the electron diffusion coefficient
$D_p$ is the hole diffusion coefficient
$\mu_n$is the electron mobility, and $\mu_p$ is the hole mobility.

## III. Characterization Criteria for Solar Cells

The peak power, Pmax, ($J_{sc}$), ($V_{oc}$), and (FF) are the primary metrics used to assess the efficiency of solar cells. The illuminated J V characteristic curve, as shown in Figure (2), is used to determine these parameters. These parameters are used to calculate the conversion efficiency(Ƞ). For a simple p-n junction device.
Figure (2) displays the usual characteristics of a solar cell's (J - V) ( current-voltage) under lighting The highest power point is the point on the J-V curve ($J_{mpp}$,$V_{mpp}$) where the cell's power output is the greatest.

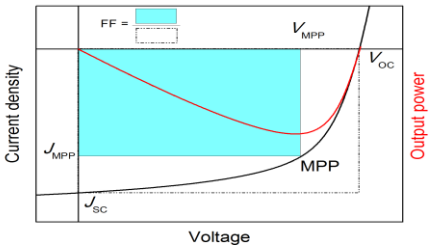


Fig.(2)( $J_{mpp}$ ,$V_{mpp}$) characteristics of a solar cell under illumination.

The solar cell's efficiency (PCE) ratio is the high output ratio (Pout = $J_{mpp}V_{mpp}$) to power input (Pin).

## IV. Model of the Device

SCAPS-1D software is used to create the device model. Figure (3) depicts the configuration of the perovskite solar cell employed in this simulation. It is a four-layered planar heterojunction structure.

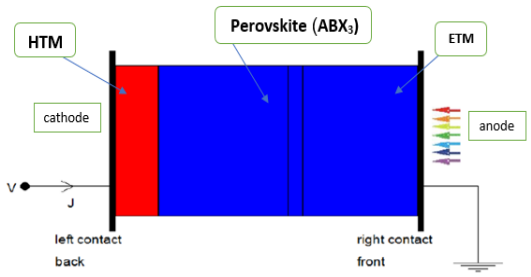


Fig.(3) Perovskite solar cell structure

Typically, there are two fundamental device structures: normal and inverted. The overall cell structure is made up of many layers that are packed on top of the FTO glass.
The SCAPS parameters for each layer and interface must be specified here. It must be established. The simulation parameters are based on practical work and theoretical research. Table (1) (a) and (b) summarize the major material and defect parameters.

**Table 1(a)**: The numerical analysis of materials parameters [5]

| parameters | FTO | $MAPbBr_3$ | $MAPbI_3$ | $MAPbCl_3$ | PCBM | $TiO_2$ |
|---|---|---|---|---|---|---|
| Band gap(ev) | 3.500 | 2.330 | 1.550 | 1.550 | 2.000 | 3.200 |
| Electron affinity (ev) | 4.000 | 3.700 | 3.750 | 3.900 | 3.900 | 4.100 |
| Dielectric permittivity | 9.000 | 7.500 | 6.500 | 6.500 | 3.900 | 9.000 |
| CB effective density of states ($1/cm^3$) | 2.200E+18 | 1.000E+21 | 2.200E+13 | 2.200E+18 | 2.540E+21 | 2.200E+18 |
| VB effective density of states ($1/cm^3$) | 1.800E+19 | 1.000E+12 | 2.200E+12 | 1.800E+19 | 2.540E+21 | 1.000E+19 |
| Electron thermal velocity(cm/s) | 2.000E+7 | 1.000E+7 | 1.000E+7 | 3.000E+7 | 2.000E-2 | 1.000E+7 |
| Hole thermal velocity(cm/s) | 1.000E+7 | 1.000E+7 | 1.000E+7 | 3.000E+7 | 2.000E-2 | 1.000E+7 |
| Electron mobility ($cm^2/v.s$) | 2.000E+1 | 2.400E+1 | 2.000E+0 | 1.600E+0 | 3.400E+2 | 2.000E+1 |
| Hole mobility ($cm^2/v.s$) | 1.000E+1 | 2.400E+1 | 2.000E+0 | 2.000E-1 | 1.000E+1 | 1.000E+1 |

**Table 1(b)**: HTM layer material parameters [5]

| parameters | FTO | $MAPbBr_3$ | $MAPbI_3$ | $MAPbCl_3$ | PCBM | $TiO_2$ |
|---|---|---|---|---|---|---|
| Band gap(ev) | 3.500 | 2.330 | 1.550 | 1.550 | 2.000 | 3.200 |
| Electron affinity (ev) | 4.000 | 3.700 | 3.750 | 3.900 | 3.900 | 4.100 |
| Dielectric permittivity | 9.000 | 7.500 | 6.500 | 6.500 | 3.900 | 9.000 |
| CB effective density of states ($1/cm^3$) | 2.200E+18 | 1.000E+21 | 2.200E+13 | 2.200E+18 | 2.540E+21 | 2.200E+18 |
| VB effective density of states ($1/cm^3$) | 1.800E+19 | 1.000E+12 | 2.200E+12 | 1.800E+19 | 2.540E+21 | 1.000E+19 |
| Electron thermal velocity(cm/s) | 2.000E+7 | 1.000E+7 | 1.000E+7 | 3.000E+7 | 2.000E-2 | 1.000E+7 |
| Hole thermal velocity(cm/s) | 1.000E+7 | 1.000E+7 | 1.000E+7 | 3.000E+7 | 2.000E-2 | 1.000E+7 |
| Electron mobility ($cm^2/v.s$) | 2.000E+1 | 2.400E+1 | 2.000E+0 | 1.600E+0 | 3.400E+2 | 2.000E+1 |
| Hole mobility ($cm^2/v.s$) | 1.000E+1 | 2.400E+1 | 2.000E+0 | 2.000E-1 | 1.000E+1 | 1.000E+1 |

The values of the most relevant cell parameters required for the simulation are shown in Table (1). These numbers have been chosen based on reasonable forecasts of theoretical considerations, experimental data, and current literature. The majority of the absorber characteristics and the thicknesses of the other layers were obtained from the literature [5]

## V. RESULTS AND DISCUSSION

### A. *Electron Transporting Materials*

$TiO_2$ and PCBM are semiconducting materials that can also collect some of the solar spectrum. Because of their appropriate band gap, electron affinity, wide surface area, simple abundance, and processability. they are used in solar cells for the transportation of photoelectrodes and electrons (ETM). The simulation work in this regard focuses on a comparative examination of perovskite with two distinct transparent conducting ($TiO_2$ and PCBM) as ETMs. This research aids in the refinement and development of the existing module, as well as the realization of the function of two independent optoelectronic ETMs.Very close results were achieved when using $TiO_2$, PCBM as ETM layer. The results of TiO2 were slightly better than PCBM, as shown in Table (2).

**Table (2)**: The highest efficiencies for different HTM and ETM

| parameters | Sipro-OMeTAD | $Cu_2O$ | PEDOT:PSS | P3HT |
|---|---|---|---|---|
| Band gap(ev) | 3.200 | 2.17 | 2.200 | 2.000 |
| Electron effinity (ev) | 2.100 | 3.20 | 2.900 | 3.200 |
| Dielectric permittivity | 3.000 | 7.11 | 3.000 | 3.000 |
| CB effective density of states ($1/cm^3$) | 2.500E+18 | 2.02E+17 | 2.200E+15 | 1.000E+20 |
| VB effective density of states ($1/cm^3$) | 1.800E+19 | 1.10E+19 | 1.800E+18 | 1.000E+20 |
| Electron thermal velocity(cm/s) | 1.000E+7 | 1.000E+7 | 1.000E+7 | 3.700E+6 |
| Hole thermal velocity(cm/s) | 1.000E+7 | 1.000E+7 | 1.000E+7 | 2.000E+7 |
| Electron mobility ($cm^2/v.s$) | 2.000E-4 | 2.000E+2 | 1.000E+1 | 1.000E-4 |
| Hole mobility ($cm^2/v.s$) | 2.000E-4 | 8.000E+18 | 1.000E+1 | 1.000E+0 |

Therefore, it was decided to adopt the results of the $TiO_2$ simulation only for the discussion.
With increasing thickness, the solar cell characteristics, particularly Jsc and PCE, increase more sharply up to 500 nm and very slowly beyond 600 nm. The results reveal that a thickness of 500 nm is also enough for effective photovoltaic activity. Because the absorber is the most important component of the solar cell, the quantity of light hitting it, the absorption range, and the absorber thickness all influence the pace of photogeneration of charge carriers. Due to a rise in series resistance, photovoltaic performance steadily improves beyond this thickness to 700 nm in both cases. $TiO_2$ is shown to be more sensitive than PCBM. VOC being almost constant suggests the least amount of recombination in perovskite. At 400 nm absorber thickness, the solar cell performance in the case of TiO2 as ETM is PCE =22.46 percent, VOC =1.0577 V, JSC =28.070267 mA/cm2, FF =75.64 percent

### B. *A Comparison Of Different Hole Transporting Materials*

$Cu_2O$,P3hT, Spiro-MeOTAD and PEDOT:PSS are P-type semiconductors They all have a pretty large band gap. Cu2O, P3hT, Spiro-MeOTAD, and PEDOT:PSS have band gap energies of 2.17, 2.0, 3.2, and 2.20, respectively. As shown in Fig(4), all P3hT, TiO2, and MAPbX3 have a suitable valance band location, and their valance band offset values are less than 0.1 eV.Furthermore, $Cu_2O$ has a high

hole mobility of up to 80 cm2. V-1S-1, for the reasons stated above, it is considered that all of them are possible alternative materials that can be used in HTM layers. The simulations are performed here utilizing four different types of hole carrying materials ($p_3$ht, PEDOT:PSS, $Cu_2O$, and Spiro-MeOTAD).

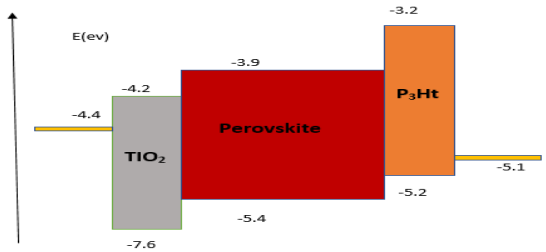


Fig. (4): Energy level diagram of $Tio_2$,p3ht and perovskite in the device.

The findings of the simulation are seen in Fig. (5) and Table(4) Fig. (5) shows J-V properties for perovskite solar cells with various HTM layers, such as $Cu_2O$, P3hT, PEDOT:PSS and Spiro-MeOTAD .

Table (3) displays the device performance data for several HTM layers, including Isc, Voc, FF, and PCE. The simulation findings clearly demonstrate that the device using P3hT as the HTM outperforms Cu2O, PEDOT:PSS, and Spiro-MeOTAD. The PCE of the gadget hits 22.46 percent when P3hT is used as the HTM. P3hT also has a relatively high Jsc of 28.070267 mA/cm$^2$ and Voc of 1.0577 V . These simulation findings demonstrate that P3hT is a likely material to be employed as a hole conveyance material.

**Table(3)**: Device performance for different HTMs

| HTM layer | Voc(v) | Jsc (mA/cm$^2$) | FF% | PCE% |
|---|---|---|---|---|
| $Cu_2O$ | 1.1250 | 25.846588 | 71.13 | 20.68 |
| spiro-OMeTAD | 1.1212 | 25.957705 | 71.36 | 20.77 |
| P3hT | 1.0577 | 28.070267 | 75.64 | 22.46 |
| PEDOT:PSS | 1.0902 | 26.963924 | 70.92 | 20.85 |

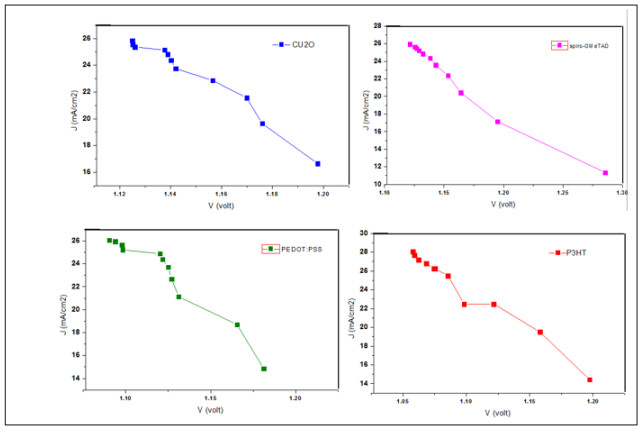


Figure (5): J-V characteristics for different HTMs

### C. *The Effect of Thickness of the Perovskite Layer on the Solar Cell*

The thickness of the perovskite has been changed from 100nm to 1300nm, with the HTM layer being $Cu_2O$/spiro-OMeTAD/$P_3$hT/PEDOT:PSS and the ETM layer being PCBM/$TIO_2$. It has been discovered that increasing the perovskite layer thickness increases the efficiency of the solar cell up to a specific point, which is thought to be the ideal thickness for the solar cell, and that doing so beyond that point decreases the efficiency.

According to the modeling, a thickness of 600nm–700nm will be adequate to almost absorb AM 1.5G radiation. As illustrated, a thick coating of 650 nm absorber is appropriate for high PCE in perovskite solar cells. It was the lowest perovskite efficiency of $MAPbBr_3$ due to its large band gap (2.33). As in the table and figure below.

**Table (4)**: device parameters for different HTM layer for $MAPbBr_3$

| HTM layer | Voc(v) | Jsc (mA/cm$^2$) | FF% | PCE% |
|---|---|---|---|---|
| $Cu_2O$ | 0.2103 | 14.090323 | 38.03 | 11.27 |
| spiro-OMeTAD | 0.3518 | 11.765198 | 22.73 | 9.41 |
| P3hT | 0.2298 | 14.405182 | 34.80 | 11.52 |
| PEDOT:PSS | 0.4716 | 8.863652 | 16.86 | 7.05 |

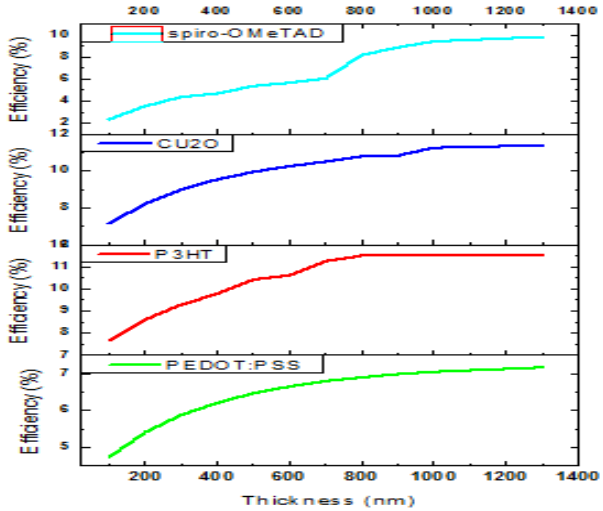


Fig.(6): showing the low $MAPbBr_3$ efficiency with the difference of HTL.

From the figure, we can see that the highest efficiency we got was when using P3hT as HTL and it was (11.52).

As for $MAPbCl_3$ and $MAPbI_3$, their results were very close, and the reason for that is the similarity of the band gap for them. As shown in Figure (7).

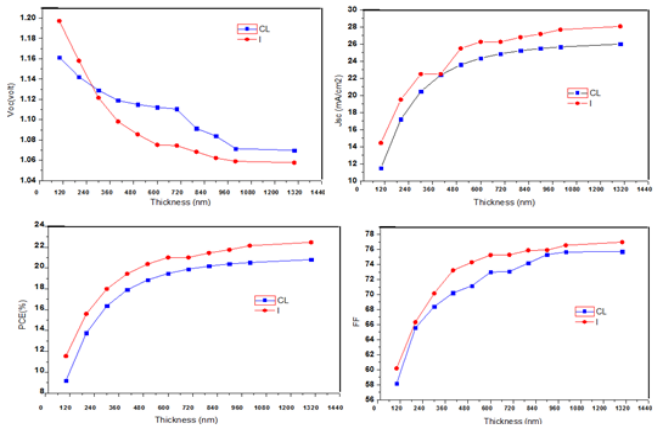


Figure (7 ): The variation of Jsc, PCE, FF, Voc versus the thickness of $MAPbI_3$,$MAPbCl_3$

As seen in Figure (7), Jsc increases with thickness, which is attributable to the production of additional electron-hole pairs in the perovskite, resulting in an improvement in efficiency. MAPbI3 has the maximum efficiency of 22.46 percent. However, efficiency stability or a tiny increase in the thicker absorber layer is owing to a lower electric field, which changes the charge carriers' recombination behavior within the absorber.

## VI. Conclusions

In this study, the thickness of the perovskite layer (from 100 to 1300 nm), we altered the electron transporting materials, thickness of the Perovskite Layer and reached the highest efficiency of 22.46% and JSC=28.070267mA/cm2 at thickness (200 nm for $TiO_2$,100 nm for P3hT,700 nm for $MAPbI_3$), and we found that the optimum value of efficiency corresponding to value of VB and CB (CB=2.20E13,VB=2.200E12 for $CH_3NH_3PbI_3$ ) at temperature 263.15 K

## Conflict of interest

Authors declare that they have no conflict of interest.

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