Pak. Sci. Bull. ISSN 2958-6747
Volume 1 issue 2 ,2022

SIMULATION STUDY ON HIGHLY STABLE HOLE TRANSPORT LAYER-BASED LEAD HALIDE PEROVSKITE SOLAR CELL

Rimsha bibi[1], Anis Naveed, Aroosa Bibi, M. Abrar[2], Mohammad Hatamvand[4], ***Irfan Ahmed[1,2,3]*,***

[1]Department of Physics, Government College, Balakot, 21300 Mansehra, Khyber Pakhtunkhawa, Pakistan

[2]Department of Physics, Hazara University, 21300 Mansehra, Khyber Pakhtunkhawa, Pakistan

[3]Center of Micro-Nano System, School of Information Science and Technology (SIST), Fudan University, 200433, Shanghai, China.

[4] Key Laboratory of Flexible Electronics (KLoFE) & Institute of Advanced Materials (IAM), Nanjing Tech University (Nanjing Tech), 30 South Puzhu Road, Nanjing 211816, Jiangsu, China

sswateez.scme.nust@gmail.com.

ABSTRACT

Cesium lead iodide ($CsPbI_3$) has been considered a promising addition to inorganic halide perovskite for its durability and potential to gain efficiency. However, to take maximum advantage of its optoelectronic features, a deep understanding of its structure and the working mechanism is necessary, which has not been the case so far. In the present study, we modeled a perovskite solar cell device using SCAPS-1D to investigate efficiency limit of $CsPbI_3$as photo absorber, and the factors affecting its performance parameters. Studies have revealed that Spiro-OMeTADas Hole Hole Transporting Layer (HTL) and TiO_2as Electron Transporting Layer (ETL) are the best suitable material for these device architectures. Thus, we have incorporated these materials for their respective functions. In addition, device performance was also observed by varying various parameters such as; work functions of the rear electrode, absorber layer thickness as well as defect density of photoabsorber layer. Under improved conditions, 23.62% conversion efficiency was achieved FTO / TiO_2 / $CsPbI_3$ / Spiro-OMeTAD PSC, indicating that there is plenty of room for further performance enhancement.

Key Points: Perovskite Solar Cells (PSC), Absorber, Photovoltaic (PV), Simulation, SCAPs-1D,

1. INTRODUCTION

Energy is the elementary requirement for human life and its consumption is growing day by day through human and industrial development (Yilmaz and Atmanli 2017). Sources from which energy is being taken are divided into three major categories: Residual Oil, Renewable and Nuclear resources. Renewable energy resources that can be useful in generating energy and are constantly occurring in the natural environment. For an instance, sunlight, wind energy, biomass energy, geothermal energy, etc. (Panwar, Kaushik, and Kothari 2011). Solar energy is utilized through photovoltaic cells generally known as solar cells. Solar cells are of two types, namely wafer based cell (WBS) and thin film-based cell (TFBC). Barriers to the WBS are low absorption coefficient, cost inefficiency, and poor performance at elevated temperatures and low light conditions. To overcome such barriers, a perovskite TFBC with high absorption coefficient, flexibility and efficiency enhanced at high temperature and low light conditions was introduced. (Sahoo, Manoharan, and Sivakumar 2018). TFBC most of the material in this phase has not yet been used commercially and many materials are still in use in research or under the development phase. The efficiency of the perovskite solar cell (PSC) has been steadily rising for a decade from 3.8% to 25.7%(Min *et al.*,2021). These technologies include Quantum dot, organic PV, and perovskite. The PSC was reported to have 9% efficiency in 2009, which increased significantly in the following years and reached to majestic height of 25.7% in relatively a short time span. Global research aims to apply their optoelectronic features and study the effects of various boundary modifications (bandgap, mobility, layer thickness etc.) on efficiency and stability. Such high performance is attributed to the optical high coefficient of absorption and the chargeable modes of transport with the length of the distribution length(Jung and Park 2015). In PSC, the device architecture consisting of 5 layers, including Transparent Conductive Oxide (TCO), Electron Transport Layer (ETL), Perovskite Absorbing Material, Hole Transport Layer (HTL) and both Metal Electrodes (Olaleru *et al.*,2020).

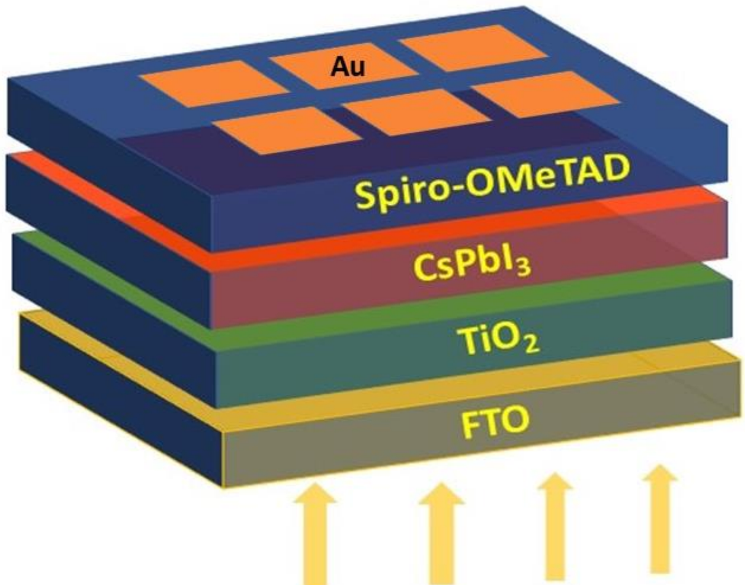

Figure 1: The generalized structure of perovskite solar cell (PSC) consisting of a transparent conductive oxide (TCO), an electron transport layer (ETL), a light absorbing perovskite material, a hole transport layer (HTL) and a metal electrode.

ETL and HTL play an important role in the extraction and transport of electrons and holes created by light absorption through the perovskite layer of the solar cell (Roy *et al.*,2020).Various device structures and production processes are subject to research and development to improve PSC's performance and reduce their future barriers of commercialization. Numerous techniques have been adopted such as doping, blending materials, formulation of Formamidinium and Cesium Lead Iodide Solid-State Alloys replacing organic living molecules [Active and Stable $CsPbI_3$ for $CsPbI_3$ Perovskite Solar Cells Exchange Process] to achieve these goals(Rong *et al.*,2018).

$MAPbI_3$, $FAPbI_3$, $CsPbI_3$ are some perovskites used in the fabrication of PSCs. $MAPbI_3$ is most common in all with very low exciton binding and strong visual absorption. But the problem with these structures is that they are rapidly affected by temperature, light and humidity and are therefore degraded in ambient condition. $FAPbI_3$is another perovskite that has improved thermal stability and a PCE of 20.09%. However, cesium based all-inorganic PSC is stable at high temperature and has an efficiency of up to 19%(Chen *et al.*,2017).

Current research focuses on one of the most promising and exploratory features currently used to improve the robust properties and high performance of cesium (Cs) PSC technology. It is the 45th most abundant element among 36 metals, more than cadmium, mercury, tin, tungsten and silver. The introduction of Cs into the hybrid perovskites can improve the thermal stability at temperatures above 100 °C, improve the visual and electrical properties, modify the crystal lattice to measure the thermodynamic phase durability, precisely control the film formation, improve the performance and performance of devices, etc. In addition to the hybrid Cs-doped perovskites, their the inorganic counterparts, in which the living component is completely replaced by a Cs cation, also show interesting, further enhanced properties with the introduction of Cs to improve the visual coupling between the active and HTL components. ETL. Finally, several examples will be shown to show that Cs-based perovskites can be used in areas other than photovoltaics, such as photoluminescence probes, photodetectors, etc. (Bella *et al.*,2018). This is done in a lab or in computer simulation. Simulation software is very useful, as it saves not only time but also lab expanses. SCAPS-1D is a one-sided solar cell simulation program, which designs solar cells in one place. A number of boundary modification options are available in SCAPS-1D. The impact of each variation is easily seen and we can stack seven semiconducting layers. Although not 100% accurate but it does provide good measurement of lab results. Our study is focused on the investigations of the thickness of $CsPbX_3$ absorber layer(s) on Current Voltage (I-V), Power conversion efficiency (PCE) and fill factor (FF) using SCAPS-1D. We will select the best material thickness to get the highest quality and learn the effect of halide anions such as (Cl, Br & I) adjustment on various parameters of the modified storage device(Slami, Bouchaour, and Merad 2019a).

2. NUMERICAL SIMULATION

This study is aimed at determining the thickness and temperature effects and also defect density on performance parameter (V_{oc}, Jsc and FF) of all inorganic $CsPbI_3$ by testing them in SCAPS-1D. Following equation for its performance are used in SCAPS;

is famous Poisson’s Equation (Eq. 1), while (Eq. 2 and 3)

are the equations of continuity for hole and electrons, respectively. In above mathematical relations**(**Eq.1, 2 and 3), **ψ** is electrostatic potential, is diffusion coefficient, **G** is generation rate, ξis permittivity while n, p, n_t and p_t represent free electrons and holes, trapped electrons and holes respectively. $N_d^+$is ionized donor density and $N_a^-$is ionized acceptor density (Nkele *et al.*,2021).The performance parameters of a photovoltaic device (PV) device are detailed numerically (Equation 4 to 7);

$$V_{OC} = \frac{nKT}{q}\left(ln\frac{I_c}{I_o} + 1\right) \ldots\ldots (4)$$

$$J = J_o\left[\exp\left(\frac{qT}{nKT}\right) - 1\right] - J_{sc} \ldots\ldots (5)$$

V_{OC} is open circuit voltage, **J_{SC}** is short circuit current and **J_o** is saturation current density. PCE (η) is represented as below:

$$\eta = \frac{P_{out}}{P_{in}} = \frac{[FF * V_{OC} * J_{sc}]}{P_{in}} \ldots\ldots (6)$$

$$FF = \frac{V_{mp}J_{mp}}{V_{OC}J_{sc}} \ldots\ldots (7)$$

Where **V_{mp}** and **J_{mp}** are voltage and current at maximum power point respectively.

We studied the effect of varied thickness, defects density and temperature on performance parameters of FTO/TiO_2/$CsPbI_3$/Spiro-OMeTAD, architecture perovskite solar cell as shown in figure 2. We simulated cell for thickness and selected the best thickness and then varied the defects, after choosing the optimum defects, thermal conditions were tuned to study their influence on operation of photovoltaic devices. Layers parameters are extracted from the literature (Yao *et al.*,2021) (Isoe *et al.*,2020) (Sebastian and Kurian 2021) (Husainat *et al.*,2019) and are summarized in the tables below.

3. RESULTS AND DISCUSSION

The PSC designed by using SCAP-1D can be seen in figure 2. CsPbI3 is used as photoabsorber and the regular device structure was used where the light was shined through FTO side.

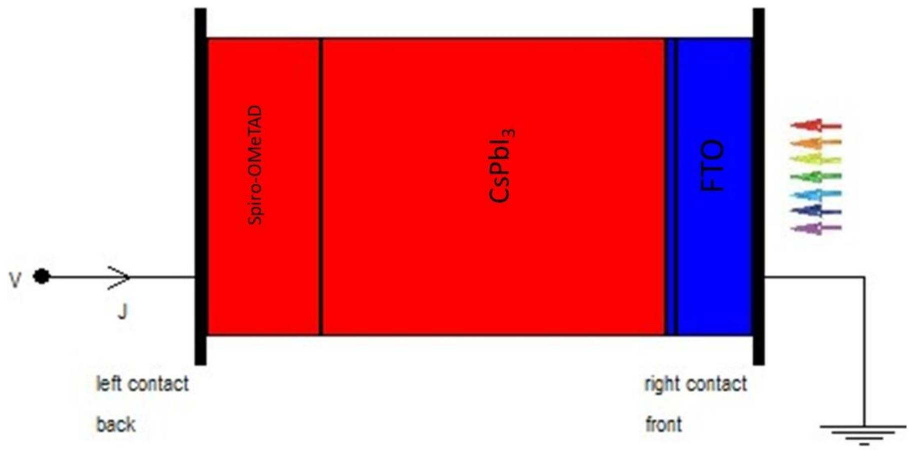

Figure2: By using SCAP-1D, the designing of various layers stacked in perovskite solar cell with $CsPbI_3$ as photoabsorber.

Similarly, various basic parameters (Table 1) were used as input parameters in SCAP-1D. these parameters are taken from extensive literature survey. Also, for the investigations of the effect of defect density on working PV device, various defect parameters are used as input parameters, as detailed in table 2.

Table 1: Parameters of layer used for simulation Perovskite Solar Cells

Sr. #	Parameters	FTO	TiO_2	$CsPbI_3$	Spiro-OMeTAD
1.	Thickness (nm)	200	30	300 varied	300
2.	Band gap, E_g (eV)	3.6	3.26	1.694	2.9
3.	Electron affinity, χ_e(eV)	4	4.26	3.950	2.2
4.	Relative dielectric permittivity, ϵ_r	9	10	6	3
5.	CB effective density, N_C(cm^{-3})	2.2×10^{18}	2.2×10^{18}	1.1×10^{20}	2.5×10^{18}

6.	VB effective density, N_D(cm^{-3})	1.80×10^{19}	1.8×10^{98}	8.2×10^{20}	1.8×10^{19}
7.	Electron Thermal Velocity(cm/s)	1×10^7	1×10^7	1×10^7	1×10^7
8.	Hole Thermal Velocity(cm/s)	1×10^7	1×10^7	1×10^7	1×10^7
9.	Electron Mobility, μ_n(cm^2/Vs)	20	20	25	2×10^{-4}
10.	Hole Mobility, μ_p(cm^2/Vs)	10	10	25	2×10^{-4}
11.	Shallow uniform donor density, N_D(cm^{-3})	1×10^{18}	5×10^{17}	0	0
12.	Shallow uniform acceptor density, N_A(cm^{-3})	0	0	1×10^{15}	1×10^{22}

Table 2: Parameters of the defect for single distribution

Sr. #	**Layer**	**FTO**	**ETL (TiO_2)**	**$CsPbI_3$**	**Spiro-OMeTAD**
1.	Defect Type	Neutral	Neutral	Neutral	Neutral
2.	Electron capture cross-section(cm^2)	1×10^{-15}	1×10^{-15}	1×10^{-15}	1×10^{-15}
3.	Hole capture cross-section(cm^2)	1×10^{-15}	1×10^{-15}	1×10^{-15}	1×10^{-15}
4.	Energetic Distribution	Single	Single	single	Single
5.	Total defect density(cm^{-3})	1×10^{15}	1×10^{15}	2.07×10^{14} varied	1×10^{15}

4. EFFECT OF PEROVSKITE($CSPBI_3$) THICKNESS:

In the current paper, we observed the effect of thickness of the perovskite layer ($CsPbI_3$) on PCE. Figure 3(a) represents the saturation value for Jsc when thickness reaches 900nm.The reason for the hike in Jsc is due the broading of the photoabsorber and further increasing its curve is straightforward(Abnavi, Maram, and Abnavi 2021). However, there is a decrease observed as the thickness increase from 300 to 1200 nm. The effect of decrease in V_{oc} is may be associated to recombination currents when thickness grows larger than diffusion length. Similarly,Figure3(b) shows increase in Fill factor with increase in thickness,probably because of increasing in Jsc(Pazos-Outón, Xiao, and Yablonovitch 2018)and it has been seen that the highest PCE has been reached at the thickness of 900 nm. For layers thicker more than 900 nm, a negligible decrease in PCE has been observed due to decrease in the electric field in the thicker perovskite layers resulting in reduced charge carrier extraction, which is proved by many experiments(Domanski *et al.*,2016).

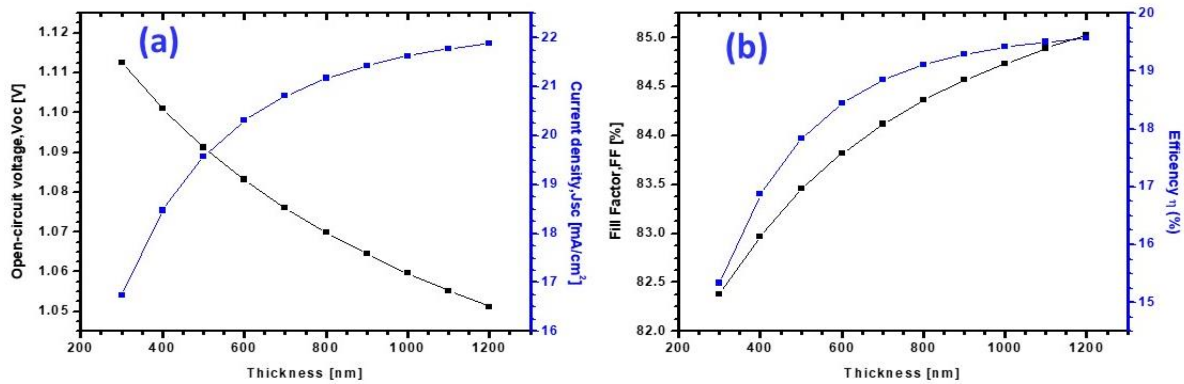

Figure3:(a) Open circuit Voltage and Current density (b) Fill factor and Efficiency as a function of $CsPbI_3$ thickness

5. DEFECT STUDY

The defect density of the absorber layer has a significant effect on perovskite solar cell performance through the configuration of photo generated carrier. Figure 4 shows the variation of PV parameters with defect density (cm^{-3}). Generation, recombination, the transport process takes place with in the absorber layer, so the quality of the absorber layer and the parameters of the defect significantly affect the performance of the device. These defects influence carrier recombination, reduction in lifetime and carrier mobility(Abnavi, Maram, and Abnavi 2021) . In the simulation model, the defect density varied from$1.57x10^{12}$ cm^{-3} to $7.03x10^{14}cm^{-3}$.It was noted that, if the defect density of absorber layer is increased from $1.57x10^{12}$ cm $^{-3}$ to 7.03x10 ^{14}cm^{-3}, a simultaneous decrease in all the photovoltaic parameters has been observed (Figure 4) and at defect density (2.07x10^{14}cm^{-3}) the PCE reaches to the 19.26 % , fill factor is 84.56 %, Voc =1.0645V and Jsc=21.432 mA/cm^{2} . When the defect density of the absorber layer element is reduced to 1.57x10^{12} cm $^{-3}$, the maximum accessible PV parameters observed are; efficiency: 23.62%, Fillfactor: 83.95%, Jsc = 21.434 mA / cm^{2}, Voc = 1.3128V. The same behavior was found in experiment (Slami, Bouchaour, and Merad 2019b)

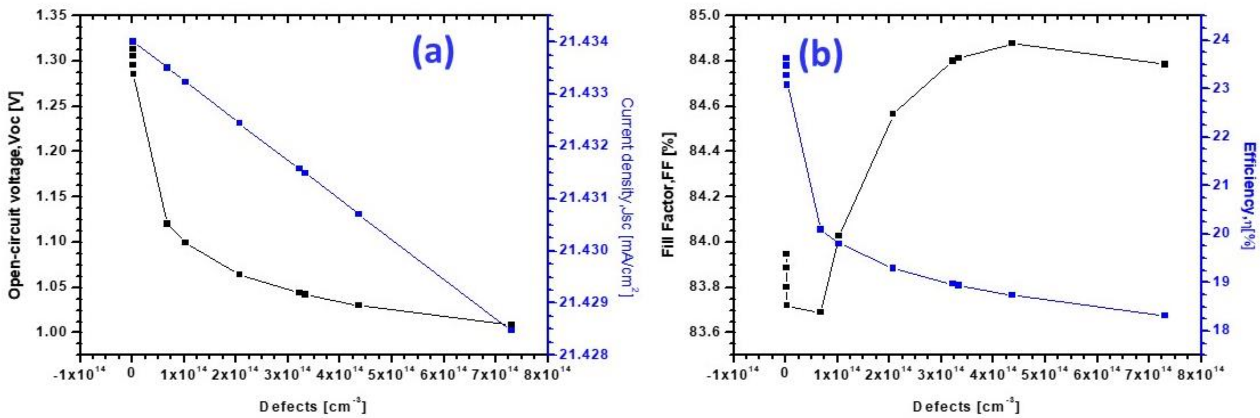

Figure4:(a) Open circuit Voltage and Current density (b)Fill factor and Efficiency as a function of defects density.

6. TEMPERATURE EFFECT ON WORKING PEROVSKITE SOLAR CELL

Temperature influences the performance of a PSC device. For understanding the effects of temperature on solar cell's electrical performance, the model temperature of simulated model was adjusted between 300 and 380K. Figure 5 reflects that any temperature increase significantly decreases the device performance. This is due to the increased resistance of the series leading to a decrease in the carrier diffusion length. As the temperature rises, the rate of recombination also increases. As a result of this at higher temperatures, the efficiency and FF decrease swiftly. As the temperature rises due to the thermal generation of charge carriers, there is a slight increase in the short circuit current density, but the decrease in open circuit voltage (OCV) is greater than the rate of increase of short circuit density and ultimately the efficiency decreases. In order to attain optimal performance, the maximum temperature of the modified model is set to 300K. (Dubey, Sarvaiya, and Seshadri 2013)

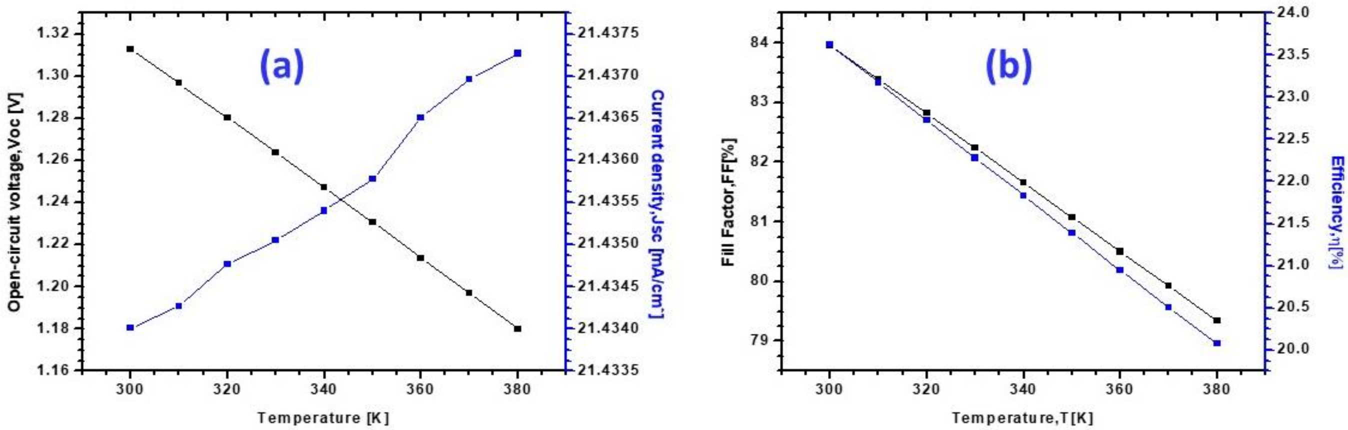

Figure5:(a) Open circuit Voltage and Current density (b)Fill factor (FF) and Efficiency as a function of temperature effect

7. CONCLUSION

The Inorganic perovskite solar cells with best thickness 900nm ($CsPbI_3$) with different parameters were analyzed by SCAPS-1D simulation software.TiO_2 material with thickness 30nm was proposed as the ETL and Spiro-OMeTAD material with thickness 300nm was proposed as the HTL for inorganic $CsPbI_3$ based PSC. The effect of thickness, defect density and temperature of absorber layer were tuned to investigate the optimized performance. Simulated results revealed that the efficiency of this solar cell is 23.62%. In future, the results will pave a way for further investigation on all-inorganic Cesium-based Perovskite solar cell which will eventually lead to commercial use of these PV devices.

8. ACKNOWLEDGEMENTS

The authors thank to Dr. Marc Burgelman at the Electronics and Information System, University of Gent, Belgium for providing SCAPS-1D simulator.

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