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Enhancing of $CH_3NH_3SnI_3$ based solar cell efficiency by ETL engineering.

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Abstract – *Solar cells based on organic-inorganic perovskites (PVK) are the subject of several researches in laboratories around the world. One of the most promising hybrid perovskite is the methylammonium lead tri-iodide $MAPbI_3$ that is suitable for sun light harvesting. But the $MAPbI_3$ is a toxic material, so in this paper is proposed another nature friendly candidate which is the methylammonium tin tri-iodide $MASnI_3$. The proposed material is inserted into an n-i-p heterojunction solar cell which structure is electron transport layer (ETL)/PVK/hole transport layer (HTL). The used HTL is the PEDOT: PSS in combination with one of two ETLs which are the PCBM and the IGZO. Simulation efforts using 1D SCAPS was carried. It is found that IGZO ETL based solar cell yields a higher power conversion efficiency (PCE) compared with PCBM ETL based solar cell in the same thickness.*

Keywords: *Perovskite, Solar cell, SCAPS Software, PCE, PCBM, IGZO.*
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NOMENCLATURE		ABBREVIATIONS	
Voc	Open circuit voltage	FF	Fill factor
Jsc	Short circuit density of current	PCE	Power conversion efficiency
E_g	Band gap energy	PVK	Perovskite
χ	Electron affinity	ETL	Electron transport material
Nc	Conduction band effective density of states	HTL	Hole transport material
Nv	Valence band effective density of states	$MASnI_3$	Methylammonium tin tri-iodide
ε_r	Relative permittivity	$MAPbI_3$	Methylammonium lead tri-iodide
μ_n	Electron mobility	PCBM	Phenyl-C61-Butyric-Acid-Methyl-Ester
μ_h	Hole mobility	PEDOT:PSS	poly(3,4-ethylenedioxythiophene) polystyrene sulfonate
N_A	Shallow uniform acceptor density	IGZO	Indium galium zinc oxide
N_D	Shallow uniform donor density		
Nt	Defect density of states		
α	Absorption coefficient		
h	Plank constant		
v	Frequency of light		
A and B	Material dependent constants		

I. Introduction

Recently, power conversion efficiency of perovskite solar cells stepped exponentially from 2.2 % in 2006 [1] up to 25.2 % in 2019 [2]. This evolution attracted researcher's attention to simulate new designs, fabricate perovskite solar cells using deferent methods and study of processing effects on device performances [3-5]. A numerical simulation has been done by researchers they find that the power conversion efficiency is 21.8% under optimized conditions and a PCE of up to 15% were obtained by initially optimizing the preparation of the layer absorbent CH3NH3PbI3 [6]. A study shows that the energy conversion yields of perovskite-based solar cells have improved significantly to over 20 %, which now makes them equivalent to the performance of silicon-based photovoltaics [7, 8]. A group of researchers found that the energy of Auerbach decreases with the rise in the temperature of the treatment giving the lower value of 0.66 eV at 100 ° C, which also corresponds to the best band range of 1 to 49 eV [9]. A numerical study has been made which focuses on the thickness and density of the states (donors and acceptors) and on the efficiency of solar cells. The results found improved the power conversion efficiency (PCE) from 11.73% to 19.58% [9]. The optimization and the thickness of the layers were also done [10, 11]. Most of perovskite solar cells use lead based materials which are not environment-friendly. In this paper, simulation efforts are conducted to study a free lead alternative of perovskite solar cells. Software used for numerical calculation is SCAPS 1D [12, 13]. The objective of our work is to show that the lead-free $CH_3NH_3SnI_3$ perovskite-based solar cell exhibited better electrical performance when using IGZO material in the ETL.

II. Device structure and methodology

Figure 1 presents the n-i-p perovskite heterojunction solar cell device that contains three layers: an electron transport layer, a perovskite layer and a hole transport layer.

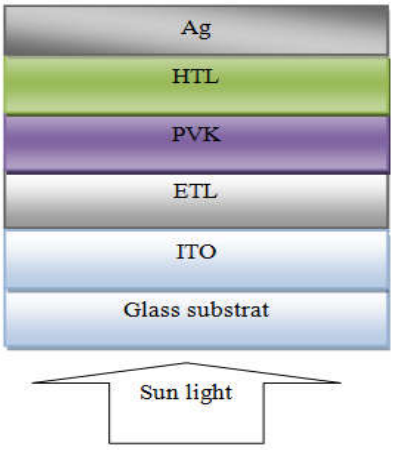

Figure 1. n-i-p solar cell structure

The Table 1 summarizes electrical and optical parameters of each layer carefully selected from literature. The solar cell is exposed to a standard AM1.5 solar spectrum under an incident power density of 100 mW/cm^2. In all simulations, the pre-factor values of A and B (see equation 1.) are taken to be equal to 10^5 and 0 respectively for all used materials for calculation simplicity.

$$\alpha=(A+B/h\nu).(h\nu-E_g)^{1/2} \quad (1)$$

Where α, *h*, *v*, E_g are the absorption coefficient, Plank constant, frequency of light and the band gap respectively, and A and B are model dependent parameters [12].

Table .1. Electrical and optical parameters

	$MASnI_3$ [3]	PEDOT:PSS [3]	IGZO [4]	PCBM [4]
Thickness	Variable	Variable	Variable	Variable
E_g (eV)	1.9	1.6	3.05	2
χ (eV)	3.98	3.4	4.16	3.9
ε_r	10	3	10	3.9
Nc (cm^{-3})	10^{16}	10^{22}	$5*10^{18}$	$2.5*10^{21}$
Nv (cm^{-3})	10^{15}	10^{22}	$5*10^{18}$	$2.5*10^{21}$
μ_n (cm^2/Vs)	16.2	$4.5*10^{-4}$	15	0.02
μ_h (cm^2/Vs)	10.1	$9.9*10^{-5}$	0.1	0.02
N_A (cm^{-3})	10^9	10^{22}	-	-
N_D (cm^{-3})	10^9	-	10^{18}	$2.73*10^{17}$
Nt (cm^{-3})	10^{14}	$2.5*10^{15}$	10^{15}	10^{15}

Figure 2 presents energy band alignment of different used materials.

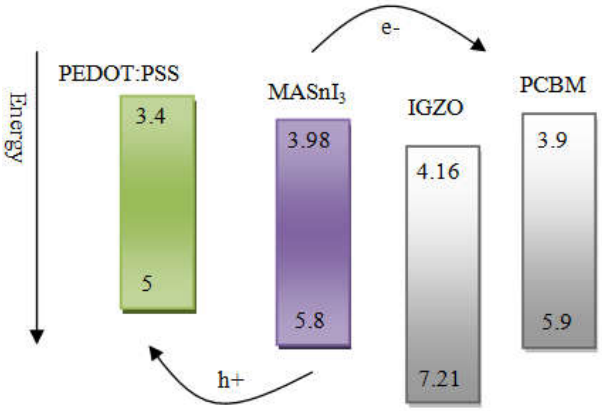

Figure .2. Energy band alignment

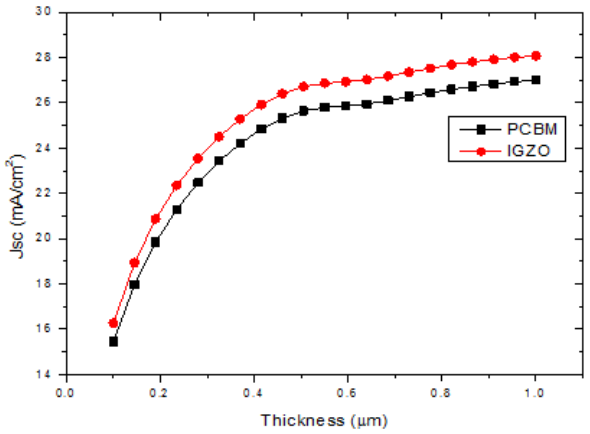

Figure .4. Short circuit density of current in function of perovskite layer thickness

III. Result and discussions

The first simulated structure is PCBM/$MASnI_3$/PEDOT:PSS/Ag with initial layer thickness of 30 nm, 400 nm and 30 nm respectively, and then we change the PVK layer thickness to find out the one corresponding to the maximum of power conversion efficiency (PCE). In the second simulated structure, we change the ETL material from PCBM to IGZO, and do the same optimization effort to find out the best PVK layer thickness that yields the maximum of PCE.

Figure 3 and Figure 4 show the different electrical parameters of both structures in function of PVK layer thickness, where we can notice that the second structure electrical parameters are better than the first structure. We can notice that concerning Voc and FF, the two structures are approximately identical. However, in PCE and Jsc curves, we can notice that in low thickness values the two structures are approximately identical but in high values there is a more difference.

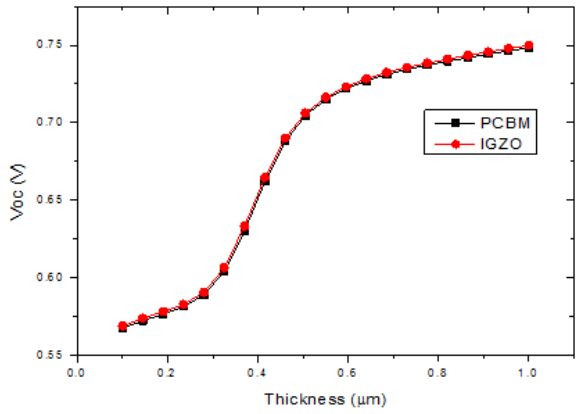

Figure .3. Open circuit voltage in function of perovskite layer thickness

Figure 5 and Figure 6 show the maximum values of the power conversion efficiency which are 12.58 % and 13.12 % for the first structure and the second structure respectively. This PCE optimized value corresponds with the PVK layer thickness of 1 µm.

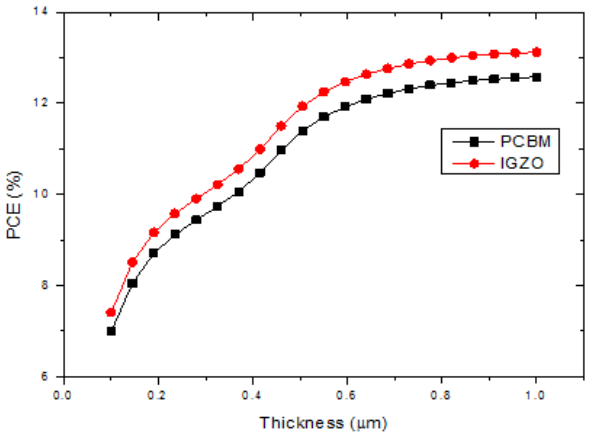

Figure .5. Power conversion efficiency in function of perovskite layer thickness

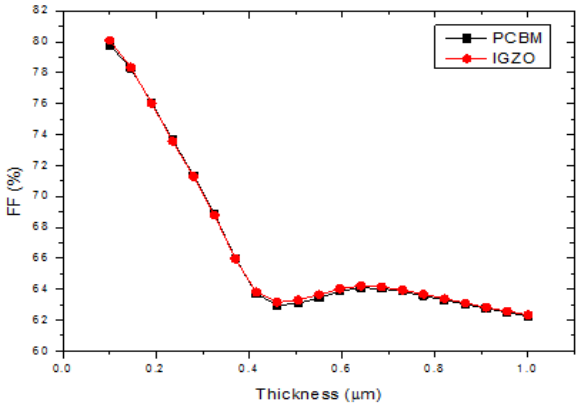

Figure .6. Fill factor in function of perovskite layer thickness

Table 2 gives the electrical parameters for both optimized structures (with PVK layer thickness of 1 µm).

Table .2. Optimized electrical parameters for both structures

Paramater	Voc (V)	Jsc (mA/cm^2)	FF (%)	PCE (%)
1st structure	0.75	27	62.25	12.58
2nd structure	0.75	28.08	62.33	13.12

Figure 7 is presents the IV characteristic of both optimized structures where it is clear that IGZO based structure is better than the PCBM structure.

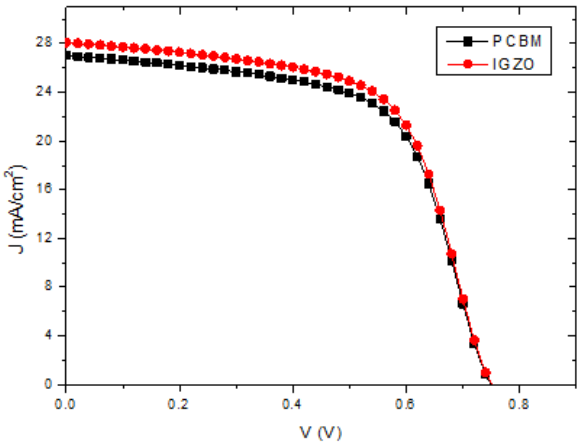

Figure .7. IV characteristics of the 1st and 2nd structures

IV. Conclusion

In this paper it is found that lead free perovskite $CH_3NH_3SnI_3$ based solar cell exhibited better electrical performances when using IGZO material as ETL. The PCE of IGZO based structure is better than the PCBM one especially in high perovskite layer thickness. It is found that IGZO based solar cell maximum PCE corresponds with 13.12 % which is better than the PCBM based solar cell maximum PCE of 12.58% with a thickness of 30 nm for both ETL and HTL, and 1 µm for $CH_3NH_3SnI_3$.

Acknowledgements

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