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Simulation and optimization of $CH_3NH_3PbI_3$ based inverted planar heterojunction solar cell using SCAPS software

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Abstract – *In order to improve the efficiency of a planar heterojunction organic-inorganic solar cell, this work is carried out using SCAPS software. The studied inverted P-I-N structure is PEDOT:PSS/ $CH_3NH_3PbI_3$/ PCBM where PEDOT:PSS is the hole transporting layer (HTL), $CH_3NH_3PbI_3$ is the Perovskite absorber layer (PVK) and PCBM is the electron transporting layer (ETL). The simulated structure is sandwiched between SnO_2: FTO and Al which are the transparent and aluminum electrodes respectively. Simulation efforts are focused on thickness and density of states (donor's and acceptors) effect on solar cell efficiency. Found results improved the power conversion efficiency (PCE) from 11.73% up to 19.58 %.*

Keywords: *Perovskite, $CH_3NH_3PbI_3$, SCAPS, power conversion efficiency, layer thickness*
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I. Introduction

From 2009 up to 2016, perovskite based solar cell efficiency stepped from 3.8 % to 22.1% [1-3]. This exponential development of perovskite based solar cell efficiency encouraged researchers to use deferent processing methods to enhance it. Due to experiment high costs, a simulation effort is a good way to calculate the better parameters prior to do experiments [4-6].

In this work we investigated effect of different layer thickness and density of states on power conversion efficiency of a P-I-N inverted planar heterojunction solar cell using the organic/inorganic perovskite material $CH_3NH_3PbI_3$ as absorber layer.

II. Device simulation parameters

Figure 1 shows deferent layer deposition of the simulated P-I-N inverted planar heterojunction $CH_3NH_3PbI_3$ based solar sell. We can see in Figure 1 the SnO_2: FTO/ PEDOT: PSS/ $CH_3NH_3PbI_3$ / PCBM where the ETM layer is the PCBM and the HTM layer is the PEDOT:PSS. In Table 1 is presented initial simulation electrical parameters that were carefully selected from practical and theoretical references [7-17].

Firstly, layer thickness is investigated to carry out the best thickness giving higher PCE. Secondly, density of states is investigated to find out better values that yeld high PCE.

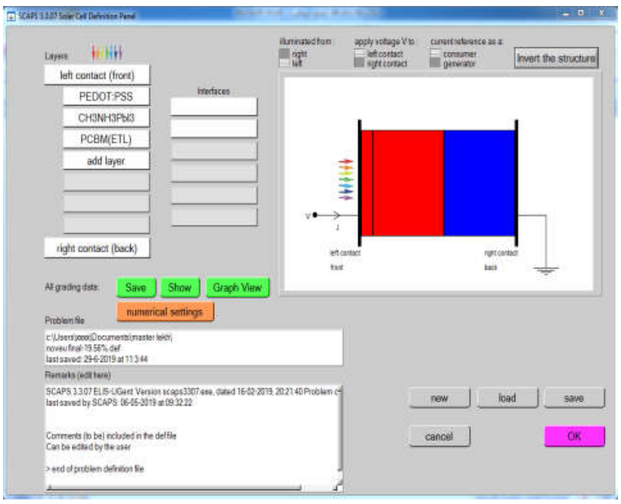

Figure 1. Planar heterojunction architecture of the studied solar cell.

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III. Results and discussion

In simulation process, the thickness of each layer was fixed in the initial values presented in table 1, then we changed the HTL thickness from 0.05 µm to 0.08 µm after that the PVK thickness is changed from 0.3 µm to 0.9 µm and in the last step the ETL thickness is modified from 0.3 to 0.6 µm. In each step we fix the thickness value that gives better PCE and use it in the next step.

Table 1. Simulation parameters

Property \ Layer	PEDOT/Pss	$CH_3NH_3PbI_3$	PCBM
Thickness (µm)	0.080	0.8	0.5
Band gap (eV)	2.2	1.55	2.100
Electron affinity (eV)	2.9	3.75	3.9
Dielectric affinity	3.000	6.500	3.900
CB effective density of states (cm^{-3})	2.200E+15	2.200E+15	2.200E+19
VB effective density of states (cm^{-3})	1.800E+18	2.200E+17	2.200E+19
Electron thermal velocity (cm/s)	1.00E+7	1.00E+7	1.00E+7
Hole thermal velocity (cm/s)	1.00E+7	1.00E+7	1.00E+7
Electron mobility (cm^2 / V.s.)	0.01	2.0	0.001
Hole mobility (cm2/ V.s.)	0.0002	2.0	0.002
Donor density N_d (cm^{-3})	1.000E+13	1.000E+13	1.000E+16
Acceptor density N_a (cm^{-3})	1.000E+16	1.000E+16	1.000E+13
Defect Nt (cm^{-3})	1.000E+15	1.000E+15	1.000E+15

Figure 2 presents layer thickness effect on PCE for every layer. It is found that the maximal value for PCE is 10.85 % which corresponds on 0.05 µm, 0.3 µm and 0.3 µm layer thickness for HTL, PVK and ETL respectively.

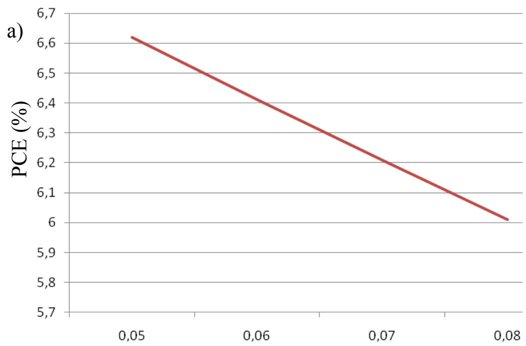

Figure 2 a. HTL Layer thickness (µm)

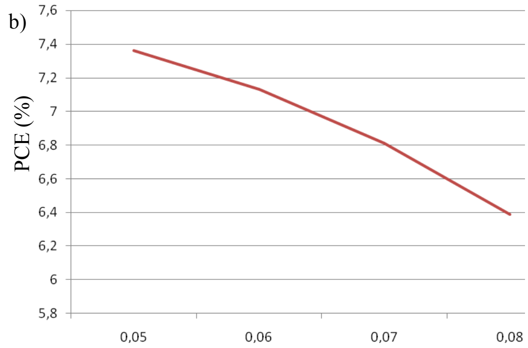

Figure 2 b. PVK Layer thickness (µm)

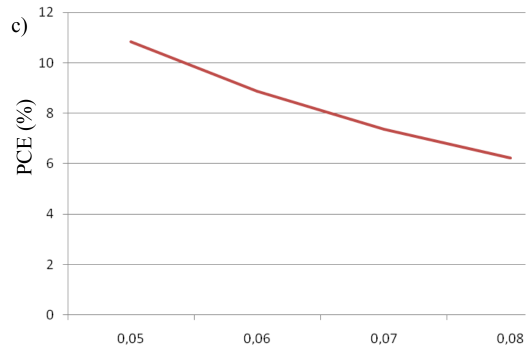

Figure 2 c. ETL Layer thickness (µm)

Figure 2. Effect of a) HTL, b) PVK and c) ETL layer thickness on PCE

The Simulation results for initial and optimized results are presented in Table 2.

Table 2. Simulation results for initial and optimized values

	Voc (V)	Jcs(mA/cm^2)	FF(%)	PCE(%)
Init Val	1.4	18.4	44.81	11.73
Opt Val	1.5	17.7	75.9	19.57

In the Figure 3 is illustrated the effect of Na of the HTL and PVK layer and Nd of the ETL layer on PCE. It is clear from curves of Figure 3 that best values that gives a PCE of 19.57 % are Na=5.10^{16} cm^{-3}, Na=5.10^{16} cm^{-3} and Nd = 5.10^{16} cm^{-3} for HTL, PVK and ETL respectively.

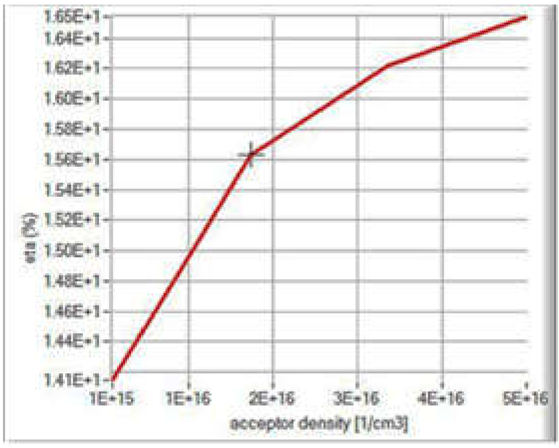

Figure 3.a

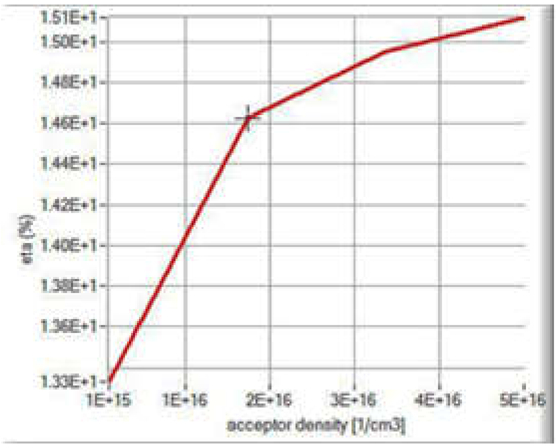

Figure 3.b

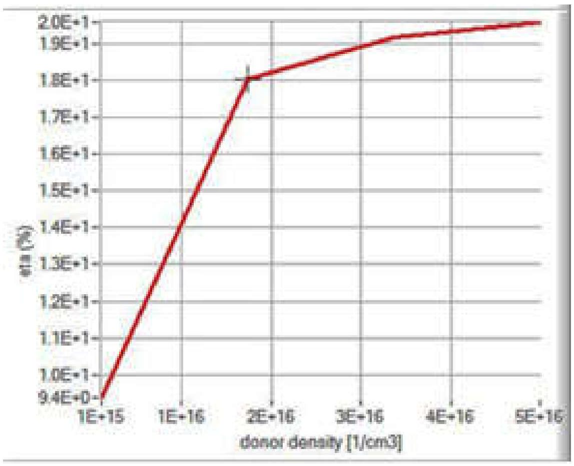

Figure 3.c

Figure 3. Effect of acceptor density of a) HTL, b) PVK and donor density of c) ETL on PCE.

IV. Conclusion

In this paper it is found that layer thickness and density of states of a P-I-N perovskite based solar cell have an important effect on PCE. Simulations done using SCAPS software have optimized the PCE of the studied structure to 19.57 % with the layer thickness values of 0.05 µm, 0.3 µm and 0.3 µm for HTL, PVK and ETL respectively, and the values of Na=5.10^{16} cm^{-3}, Na=5.10^{16} cm^{-3} and Nd = 5.10^{16} cm^{-3} for HTL, PVK and ETL respectively.

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