

Comparative study of modeling of Perovskite solar cell with different HTM layers

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ABSTRACT-The efficiency of MASnI₃ based solar cell with various hole transport material (HTM) layers including Spiro-OMeTAD, PEDOT:Pss, and Cu₂O is studied. Zinc oxide (ZnO) layer is proposed as electron transport layer for lead-free CH₃NH₃SnI₃ based Perovskite solar cells. The influence of device parameters such as doping level of the active layer, thickness of the CH₃NH₃SnI₃ layer and working temperature is discussed. For optimum parameters of all three structures, efficiency of 24.17%, 24.50%, and 25.36% for PEDOT:Pss, Spiro-OMeTAD, and Cu₂O, respectively is achieved. To study the optimized performance of this Perovskite solar cell, SCAPS-1D software is considered.

Keywords: Perovskite, CH₃NH₃SnI₃, PEDOT:Pss, Copper oxide, Spiro-OMeTAD, ZnO, HTM, efficiency, SCAPS-1D.

I. INTRODUCTION

In recent years, Perovskite oxides represent a prominent of advanced compounds involved in many areas of science and technology [JTAC 2011 1–3]. Perovskite Solar Cells (PSCs) show a great performance because of their low cost fabrication than traditional solar cells [1]. The yield of PSC increases very rapidly reaching the value of 22% [2-4]. Owing the multilayer architecture of PSCs, interface has a main role to play in performance and influences long term stability [5]. The CH₃NH₃SnI₃'s absorber layer becomes a suitable alternative of CH₃NH₃PbI₃ one because of the toxicity of this typical PSC [6].

The Spiro-OMeTAD HTM is used in organic photovoltaics (OPV) and organic optoelectronics [7], but its causes degradation in the devices performance [8]. Thus, PEDOT:Pss, or Cu₂O replace the spiro-OMeTAD HTM.

The aim of this paper is to contribute to the optimization of the efficiency of Perovskite solar cell with three different configurations: Glass/FTO/ZnO/CH₃NH₃SnI₃/HTM/Au, HTM being Spiro-OMeTAD. 1D solar cell capacitance simulator (SCAPS) is applied for this study.

II. NUMERICAL MODELLING AND DEVICE STRUCTURE

II.1. Numerical modeling

To analyze the effect of different electrical parameters on the efficiency of PCs, SnO₂:f/ZnO/CH₃NH₃SnI₃/Spiro-OMeTAD, SnO₂:f/ZnO/CH₃NH₃SnI₃/PEDOT:Pss, and SnO₂:f/ZnO/CH₃NH₃SnI₃/Cu₂O heterojunction-based perovskite solar cell structures, are adopted. SCAPS software is used for simulation. Figure 1, explains the simulation process.

SCAPS is a one dimensional solar cell simulation program developed at the department of Electronics and Information Systems (ELIS) of the University of Gent, Belgium. It allows simulating the behavior of photovoltaic structures. Since that, there are several modifications in this software such as the capability to work with crystalline solar cells (c-Si and GaAs, family) and amorphous cells (a-Si and micro-morphous Si) [9]. This simulator has the largest number of AC and DC electrical measurements which can be calculated in dark and light illumination and also at different temperatures. It (SCAPS) solves the Basic semiconductor equations in 1-Dimension under steady state condition.

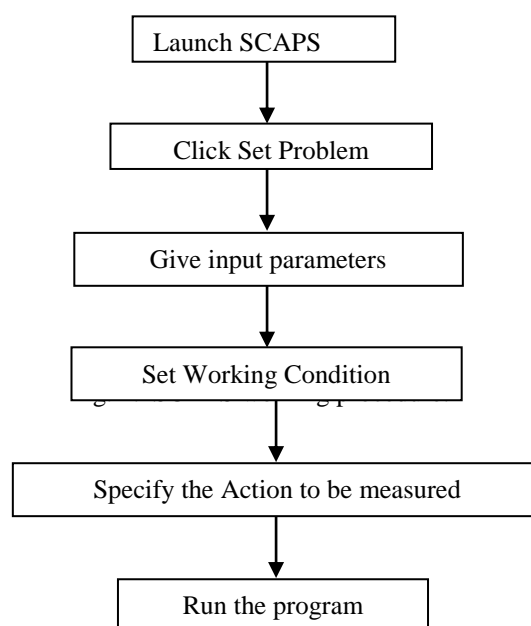


Fig. 1. SCAPS working procedure.

II.2. Device structure

The cell consists of Methylammonium tin triiodide (MASnI₃); considered as absorber layer. N-type (ZnO-ETM) is arranged

at the bottom side, and at the top three p-type (Spiro-OMeTAD, PEDOT:Pss and Cu₂O) are designed as HTM layer. figure 2 presents the three structures.

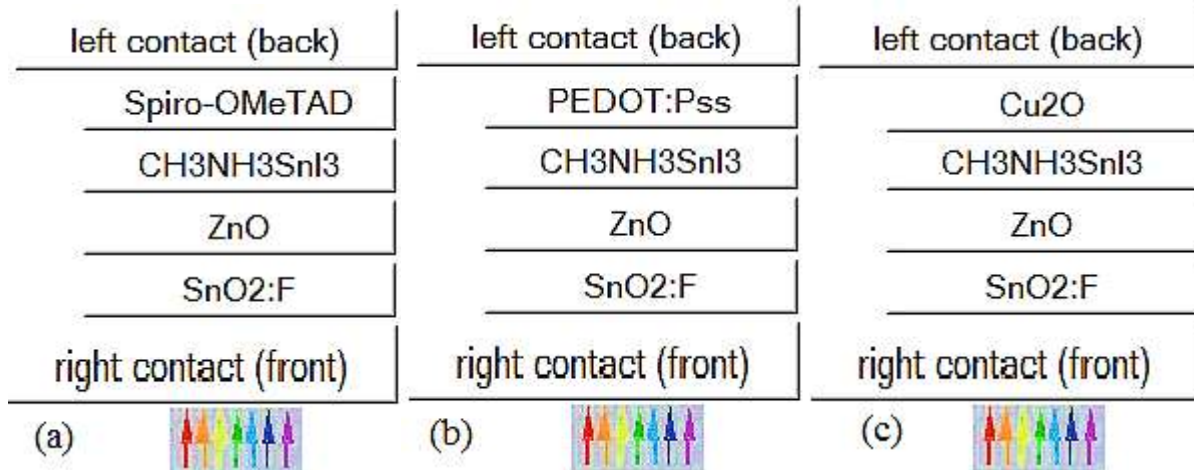


Figure 2: Schematic representation of three architectures with different HTM layers

(a) Spiro-OMeTAD(HTM)/MASnI₃/ ZnO/ SnO₂:F

(b) PEDOT:Pss(HTM)/MASnI₃/ ZnO/ SnO₂:F

(c) Cu₂O(HTM)/MASnI₃/ ZnO/ SnO₂:F

To run the simulation, SCAPS needs material parameters; in terms of bandgap (E_g), electron affinity (χ), dielectric permittivity (ϵ), conduction band density of states (N_c), valence band density of states (N_v),

electron mobility (μ_n), hole mobility (μ_p), donor density (N_D), acceptor density (N_A). Table 1 summarizes data and other theoretical results extracted from published studies.

Parameters	SnO ₂ :F [10, 11, 12]	ZnO [13-15]	CH ₃ NH ₃ SnI ₃ [16, 17-18]	SpiroOMeTAD [19-23]	PEDOT:Pss [24, 25]	Cu ₂ O [22-23]
Thickness(nm)	500	50	900	200	200	200
E_g (ev)	3.5	3.2	1.3	3.17	3.6	2.17
χ (ev)	4	4.26	4.17	2.05	1.57	3.2
ϵ_r	9	9	8.2	3	3	7.11
N_c (cm ⁻³)	2.20 x 10 ¹⁸	2.00 x 10 ¹⁸	1.00 x 10 ¹⁸	2.20 x 10 ¹⁸	2.20 x 10 ¹⁷	2.02 x 10 ¹⁷
N_v (cm ⁻³)	1.80 x 10 ¹⁹	1.80 x 10 ¹⁹	1.00 x 10 ¹⁸	1.80 x 10 ¹⁹	1.80 x 10 ¹⁹	1.10 x 10 ¹⁹
μ_e (cm ² /Vs)	20	200	1.60	2.00 x 10 ⁻⁴	10	200
μ_h (cm ² /Vs)	10	5	1.60	2.00 x 10 ⁻⁴	400	80
N_D (cm ⁻³)	2.00 x 10 ¹⁹	1.50 x 10 ¹⁷	-	-	-	-
N_A (cm ⁻³)	-	-	1.50 x 10 ¹⁶	2.00 x 10 ¹⁹	2.00 x 10 ¹⁹	2.00 x 10 ¹⁹

Table1 : Parameters used for simulation of perovskite solar cell structures using SCAPS-1D

III. RESULTS AND DISCUSSION

III.1. Influence of Absorber layer thickness

The Thickness of CH₃NH₃SnI₃ is varied from [50-900] nm with the three HTM layers (PEDOT:Pss/Cu₂O/spiro-OMeTAD) and ZnO as the ETM layer.

The simulated parameters such as Power Conversion Efficiency (PCE), Fill Factor (FF), Short circuit current density (J_{sc}), open circuit voltage (V_{oc}) of the CH₃NH₃SnI₃ solar cells, are shown in Figure 3.

All photovoltaic parameters are maximum at 900nm. The efficiency increases with increasing thickness. It will be

explained by the increase in generation of electron-hole pairs in the absorber layer. Therefore, the optical density increases. Also, with increasing thickness, the short circuit current (J_{sc}) increases because the thicker absorber layer absorbs more photons, which creates more electron-hole pairs. Moreover, with a thicker absorber layer the chance of recombination increases too; as the charges cross a long distance for diffusion [26]. The results show that the device including Cu₂O as Hole Transport Material (HTM) has the highest performance.

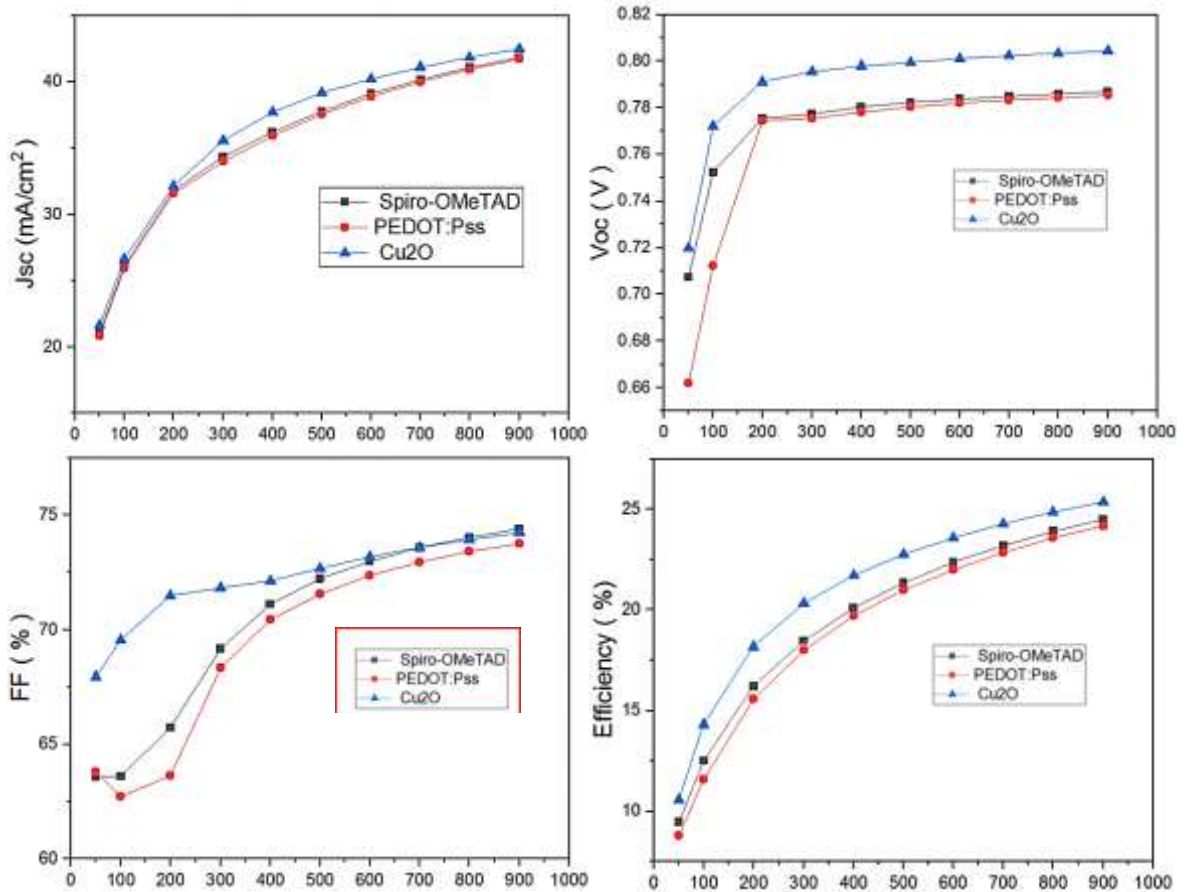


Figure 3: Variation of device performance of absorber thickness layer.

Table 2 recaps all results of PV parameters.

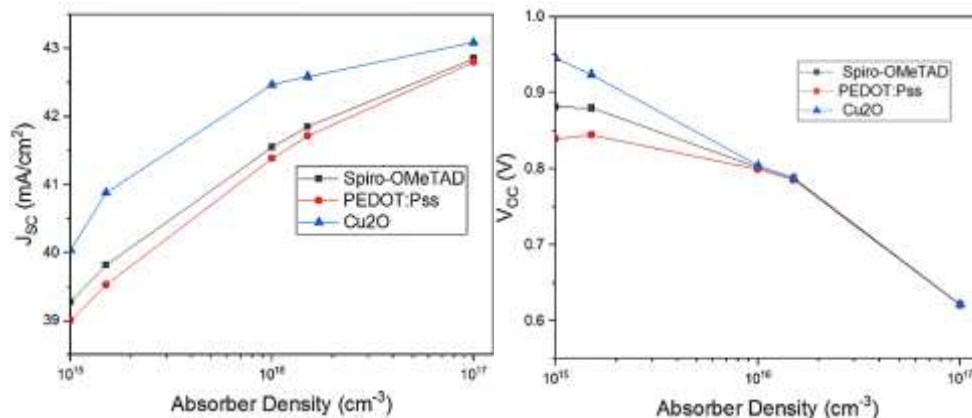
Perovskite solar cell	V _{oc} (V)	J _{sc} (mA/cm ²)	FF (%)	PCE (%)
SnO ₂ :F/ZnO/MASnI ₃ /PEDOT:Pss	0.7853	41.72	73.77	24.17
SnO ₂ :F/ZnO/MASnI ₃ /Spiro-OMeTAD	0.7868	41.85	74.41	24.5
SnO ₂ :F/ZnO/MASnI ₃ /Cu ₂ O	0.8044	42.47	74.23	25.36

Table 2: Parameters of PSC with different HTM layers.

III.2. Influence of doping of the active layers on the PV parameters

Figure 4, presents the effect of dopant concentration (doping) of Perovskite absorber layer on PV parameters. Acceptor doping concentration (N_A) is varying from 10^{15} cm^{-3} to 10^{17} cm^{-3} . The maximum value appears at N_A of $1.5 \times 10^{16} \text{ cm}^{-3}$ for both structures with HTM layers (Spiro-OMeTAD, and PEDOT:Pss). On the other hand, for structure with Cu₂O as HTM layer N_A is $1.0 \times 10^{16} \text{ cm}^{-3}$. FF changes also when N_A is varying. And all structures (SnO₂:f/ZnO/CH₃NH₃SnI₃/Spiro-OMeTAD, SnO₂:f/ZnO/CH₃NH₃SnI₃/PEDOT:Pss, and SnO₂:f/ZnO/CH₃NH₃SnI₃/Cu₂O) reach their maximum values

when the N_A is approximately $1.5 \times 10^{16} \text{ cm}^{-3}$. Hence, an appropriate doping concentration of the Perovskite absorption layer is favorable to the amelioration of the photo-absorption efficiency, J_{sc} and FF. However, the V_{oc} drops rapidly when the N_A exceeds $1.0 \times 10^{16} \text{ cm}^{-3}$ in all three considered models. Its can be explained by Auger recombination rate. Indeed, increasing doping concentration causes higher Auger recombination rate. The enhancement of the electric field is the consequence of the increase of doping concentration. This characteristic favors the separation of carriers and thus the improvement of the cell performance [21].



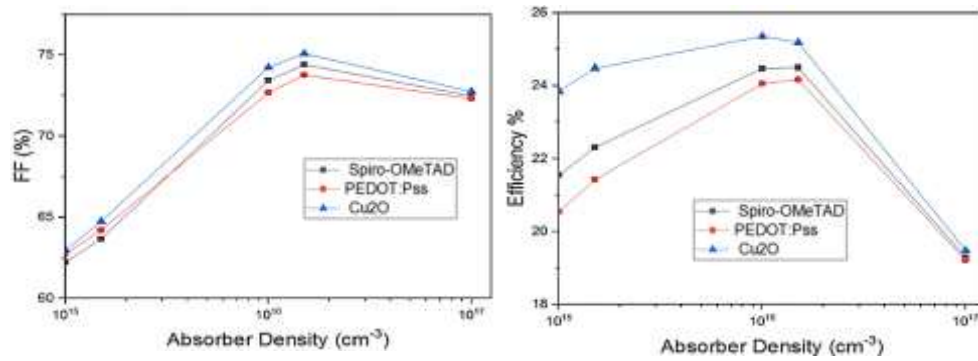


Figure 4: Effect of dopant concentrations of Perovskite absorber layer on PV parameters.

III.3. Influence of temperature

To understand the effect of temperature on the electrical performance of the solar cell, the temperature of the simulated model is changed from 300K to 450K. Figure 5 shows the variation of PCE versus temperature for all HTM layers. All the three HTM layers simulation models show similar behavior: as the temperature increases the PV parameters are decreasing not shown in this paper. As the temperature increases, defect density inside the layers increases and then reduces the efficiency. It can be explained

by the fact the defect density inside the layers increases with the temperature. It acts on deformation stress [19]. According to figure 5 ; the PSC with (Cu₂O) as HTM layer shows the better performance at high temperature (450K). Also the PSC with (Cu₂O) as HTM layer remains the more better than the two others Spiro-OMeTAD and PEDOT:Pss as HTM layers. The best operating temperature is 300K. Temperature is an important parameter; it was found that decrease in diffusion length increases of series resistance. By this fill factor and efficiency will be decreased according to papers [26-28].

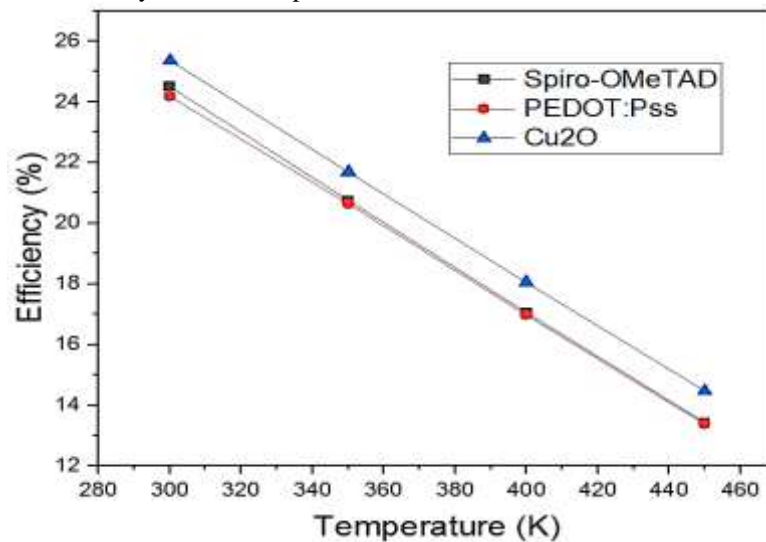


Figure 5: Effect of temperature on the efficiency

IV. CONCLUSION

In this work CH₃NH₃SnI₃ Perovskite solar cell with different parameters was analyzed using SCAPS-1D software device simulation. ZnO was suggested as electron transport layer (ETL). The performance of of PSC was studied with three different Hole Transport Material (HTM) layers (PEDOT:Pss/Cu₂O/spiro-OMeTAD). Thickness, doping and temperature, were varied to study the optimized performance.

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Results showed that solar cell containing Cu₂O as HTM outperform all other devices. A Power conversion efficiency of 25.36% was obtained. At 300K and for a thickness of 900nm for N_A=1.5 10¹⁶ cm⁻³.

In future, the results of this proposed structure need to be validated through physical fabrication and further studies.

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