Lead free organic-inorganic perovskites simulation for low toxic solar cell applications

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***Abstract*— $CH_3NH_3PbI_3$ Perovskite materials applied in organic-inorganic solar cell applications suffer from Pb toxicity. Recent researches aim to find out other alternates free lead materials. In this paper, numerical simulations of free lead perovskite $CH_3NH_3SnI_3$ have been studied and results have been presented in order to show their performances in comparison of those of $CH_3NH_3PbI_3$ using SCAPS software. The obtained results show that $CH_3NH_3SnI_3$ has better performances compared to $CH_3NH_3PbI_3$.**

Keywords—$CH_3NH_3PbI_3$, $CH_3NH_3SnI_3$, IV, power conversion efficiency, lead free perovskite

I. INTRODUCTION

In the last few years, there has been a surge of interest in the use of perovskite materials in photovoltaic solar cell research has developed exponentially [1], prompting researchers to invest in research to improve the performance of perovskite-based photovoltaic cells as well as trying to understand the various internal mechanisms that control several characteristics, including hysteresis [2, 3], power conversion efficiency (PCE) [4, 5], toxicity and stability [6-9].

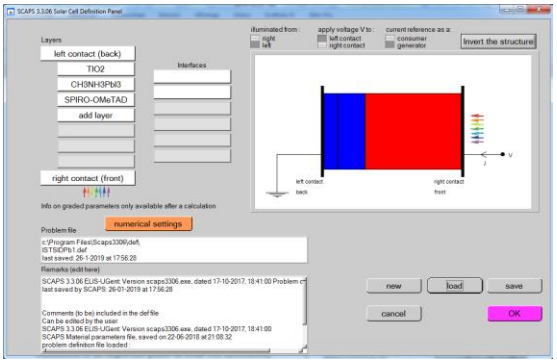
Lead (Pb) is a big problem in organic-inorganic solar cell technology because of its toxicity. Recent research are focusing in resolving this problem [10, 11]. In this paper we tried to study and simulate the performance of an alternative material which is the $CH_3NH_3SnI_3$. Therefore, two heterojunction n-i-p structure photovoltaic solar cells have been analyzed. The first structure consists the use of lead-based design and the second one is free Lead-based design. The obtained results are compared and the better ones are presented.

II. DEVICE STRUCTURE AND SIMULATION DETAILS

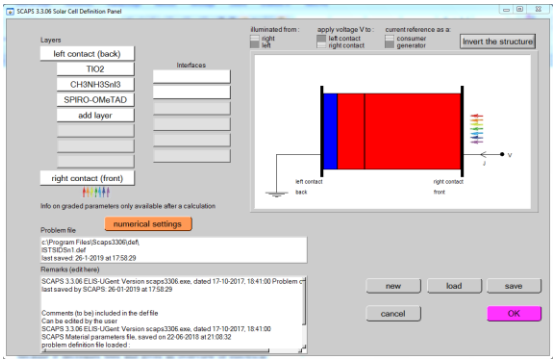
Simulation is an important phase in solar cell fabrication, because it decreases fees and gives an overview of electrical parameters enhancements. The software used in our work is SCAPS (3.3.06) software [12], which is a free software based on resolving of physical equations namely : Poisson's equation and carrier continuity equations for electrons and holes.

Figure 1 presents both structures of simulated n-i-p heterojunction solar cells, the first a) uses $CH_3NH_3PbI_3$ as absorber layer, and the second b) uses the lead free perovskite $CH_3NH_3SnI_3$ as absorber layer.

The parameters used for the simulation are summarized in table 1.



a)



b)

Fig. 1. Layer structure of a) lead-based perovskite absorber, b) free lead-based perovskite absorber.

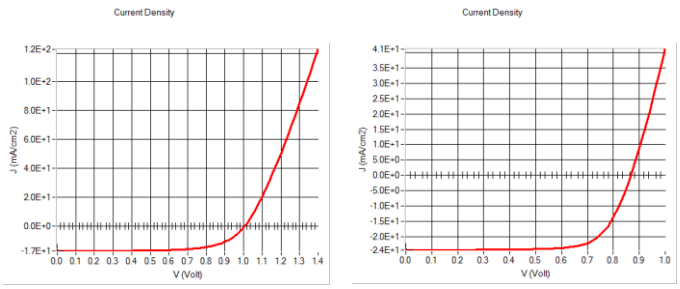
Table 1. Parameters used in simulation for both structures.

Material property	Spiro-OMeTAD	$CH_3NH_3SnI_3$	$CH_3NH_3PbI_3$	TiO_2
Thickness (nm)	700	200	200	100
Eg (eV)	3	1.3	1.55	3.2
χ (eV)	2.45	4.17	3.9	4
Nc (cm^{-3})	2.2e18	1e18	2e18	2e18
Nv (cm^{-3})	1.9e19	1e18	2e19	2e19
N_D (cm^{-3})	-	-	1e13	3e19
N_A (cm^{-3})	1e18	3.2e15	-	-
ε_r	3	8.2	100	19
μ_n ($cm^2V^{-1}s^{-1}$)	2e-4	1.6	1	0.2
μ_h ($cm^2V^{-1}s^{-1}$)	2e-4	1.6	1	0.1
τ_n (s)	1e-7	1e-6	1e-6	1e-7
τ_p (s)	1e-7	1e-6	1e-6	1e-7

Simulation parameters used in our work was carefully taken from literature, [13-16].

III. Results and Discussion

The simulation was performed using SCAPS software for both structures presented in Figure 1 and the different parameters given in table 1 have been used. Figure 2 illustrates I-V characteristics for both structures. It is noticed that lead free-based design demonstrates a better Jsc behavior in comparison with that of lead-based design. Therefore, the resulting electrical parameters such as power conversion efficiency (PCE) and fill factor (FF) are summarized in table 2.



a) b)

Fig. 2. Simulated IV characteristics of a) lead-based design, b) lead free-based design.

Table 2. Different electrical parameters found for both structures.

	$CH_3NH_3PbI_3$	$CH_3NH_3SnI_3$
Jsc (mA/cm^2)	17.15	24.30
Voc (V)	1.0051	0.87
FF (%)	67.06	73.24
PCE (%)	11.56	15.44

From results presented in table 2, it is clearly shown that the lead free structure presents a PCE and FF better than those of lead based structure, which makes $CH_3NH_3SnI_3$ a good alternative for lead free perovskite based solar cells.

IV. Conclusions

In this work, we have studied and simulated a lead free perovskite based solar cell using SCAPS software. The found results of lead free structure have been compared with those of lead based structure. It is observed that the lead free structure gives better electrical parameters namely: J_{SC}, FF and PCE than the lead based one. Therefore, in the same simulation conditions we found that the $CH_3NH_3SnI_3$ gives a better PCE by 3.88% makes it a better choice for low toxic solar cell applications.

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