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Design and Numerical Simulation of a Lead-Free Perovskite Solar Cell Using Setfos

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Abstract: The search for cost-effective, sustainable, and environmentally conscious energy alternatives is accelerating worldwide. Solar energy, as the most prominent renewable source, is set to play a crucial role in fulfilling the increasing energy needs of future generations. Despite being widely used and well-established, traditional Si solar cells have drawbacks such as relatively low absorption coefficients and high fabrication costs. Perovskite solar cells (PSCs) offer a viable solution to these limitations due to their simple bandgap adjustment, improved absorption coefficients, and lower material and production costs. To replace the toxic Pb^{2+} ions in perovskites without changing the structure of the material. Tin (Sn)-based perovskites have been becoming more prevalent among these metals over the past few decades due to their enhanced optical and electrical characteristics, including smaller bandgaps and improved charge mobility. In this study, we use a non-volatile, lead-free substance $CsSnI_3$ as the Perovskite absorber material which is an environmentally friendly artificial solution for energy-harvesting solar cell technology because of its advantageous band gap (e.g., 1.3 eV), strong visible light absorption coefficient, efficient local hole mobility, and ease of charge separation.

The proposed configuration of the Perovskite Solar Cell consists of $FTO/TiO_2/CsSnI_3/Cu_2O/Au$. Using SETFOS 5.3 simulation we optimize the thickness of each layer to achieve a PCE of 26.84%, Fill Factor of 83.59%, Open Circuit Voltage (V_{OC}) of 1.07V, Short Circuit Current Density (J_{SC}) of 29.91mA/cm^2 and External Quantum Efficiency of 85.71%. The proposed solar cell was found to exhibit 0.44% more PCE compared to the similar solar cell found in the literature.

Keywords: $CsSnI_3$, PCE, SETFOS 5.3

1. INTRODUCTION

The search for cost-effective, sustainable, and environmentally conscious energy alternatives is accelerating worldwide. Solar energy, as the most prominent renewable source, is set to play a crucial role in fulfilling the increasing energy needs of future generations. [1]. The remarkable advancements in the efficiency of renewable solar energy generation in recent years have driven the growing popularity of perovskite and thin-film solar cells as key solutions to the significant energy challenges of the 21st century. [2]. A significant area of photovoltaic (PV) technology, thin film solar cells have been thoroughly studied as replacements for conventional Si-based cells. These thin-film devices can be integrated into various applications and are lightweight and flexible. Despite being widely used and well-established, traditional Si solar cells have drawbacks such as relatively low absorption coefficients and high fabrication costs. Scientists and research teams that specialize in this industry are currently researching and making use of perovskite cells, which are a part of the third generation of solar cells. [3]. However, PSCs offer a viable solution to these limitations due to their simple bandgap adjustment, improved absorption coefficients, and lower material and production costs. [4]. The main obstacles to the mass production of PSCs were the toxicity of lead (Pb) halide perovskites, which restricts their commercial viability, and the stability of the perovskites, which rapidly deteriorate when subjected to heat, light, oxygen, or moisture. Since the outer shells of divalent metal ions, such as tin (Sn^{2+}) and germanium (Ge^{2+}), are almost equivalent to those of Pb, they can be utilized to replace the toxic Pb^{2+} ions in perovskites without changing the structure of the material. [1]. Tin (Sn)-based perovskites have been becoming more prevalent among these metals over the past few decades due to their enhanced optical and electrical characteristics, including smaller bandgaps and improved charge mobility. However, the chemical instability of the crystal structure and the discrepancy in energy levels between the absorber layer and the charge transport layer are the main drawbacks of Sn-based perovskites that keep them from achieving higher efficiencies. Thus, a non-volatile, lead-free substance $CsSnI_3$ can be used as the Perovskite absorber material [2]. $CsSnI_3$ is an environmentally friendly artificial solution for energy-harvesting solar cell technology. Because of its advantageous band gap, strong visible light absorption coefficient, efficient local hole mobility, and ease of charge separation, $CsSnI_3$ is a more advantageous lead-free inorganic perovskite material to achieve excellent device performance than lead-based hybrid perovskite materials. [5].

2. SIMULATED DEVICE STRUCTURE

Using AM 1.5G illumination spectra, SETFOS-5.3 was used to numerically investigate the efficiency enhancements of the PSC perovskite absorption layer. We examine how the PSC efficiency is affected by several optical factors, including temperature, the top and bottom electrodes' work functions, the thickness of the Perovskite Absorber Layer (PAL), the Electron Transport Layer (ETL), and the Hole Transport Layer (HTL). The device architecture and energy levels of the suggested PSC are schematically depicted in the figure. The following configuration has been suggested: FTO/TiO_2/$CsSnI_3$/Cu_2O/Au. In this case, $CsSnI_3$ is the perovskite absorber layer (PAL). The electron and hole transport layers have been selected to be TiO_2 and Cu_2O, respectively. The top and bottom electrodes of PSCs are commonly FTO and Au, respectively. Using the visible light wavelength ranging from 300 nm to 1000 nm, the simulation operates at 300K.

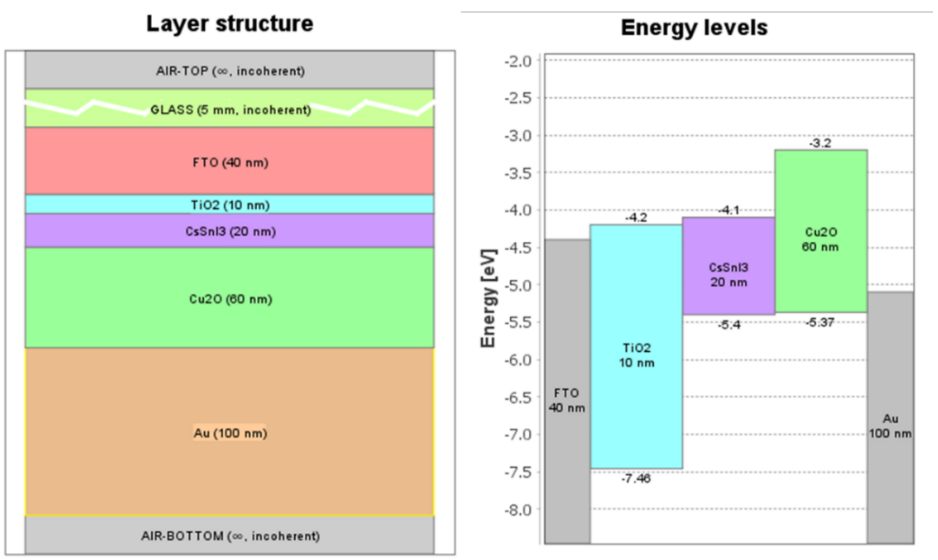

FIGURE 1. Shows the thickness and the energy levels of the Thin Film Layers used in PSC simulation.

TABLE 1: Parameters used for PSC simulation using SETFOS 5.3

	E_g (eV)	ε_r	E_H (eV)	E_L (eV)	N_H (cm^{-3})	N_L (cm^{-3})	N_A (cm^{-3})	N_D (cm^{-3})	μ_e (cm^2/V.s)	μ_p (cm^2/V.s)	REFERRENCES
TiO_2	3.26	10	7.46	4.2	2.2E18	1.8E18	0	1E17	20	10	[6]
$CsSnI_3$	1.3	18	5.4	4.1	1.47E18	1.57E19	1E15	1E15	4.37	4.37	[4], [5]
Cu_2O	2.17	7.5	5.37	3.2	1.1E19	2E18	2E19	0	20	80	[6]

3. RESULTS AND DISCUSSION

3.1 Impact of Absorber Layer Thickness on the Performance of the PSC:

The thickness of the $CsSnI_3$ PAL has been varied from 10 to 100 nm. J_{SC} grows with thickness up to 20 nm before declining due to increasing photon absorption. After a particular thickness has been achieved, V_{OC} shows variations due to higher recombination, while FF shows a range of behaviors. The PCE increases up to 20 nm, after which it falls linearly with increasing thickness. Hence, 20 nm has been chosen as the appropriate $CsSnI_3$ thickness for the upcoming simulation.

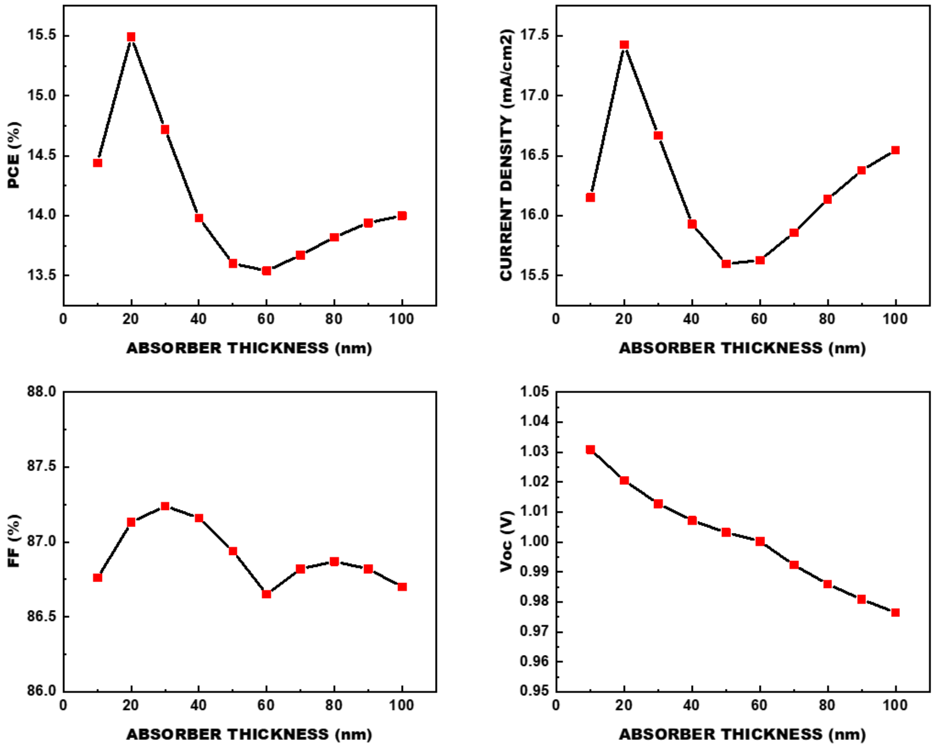

FIGURE 2. Shows how the PSC's efficiency varies as the perovskite absorber layer thickness increases.

3.2 Impact of ETL Thickness on the Performance of the PSC:

On varying the thickness of the ETL from 10 nm to 200 nm, it is found that the PCE and J_{SC} attain their maximum at 10 nm and then decreases when the thickness is increased.

3.3 Impact of HTL Thickness on the Performance of the PSC:

On varying the thickness of the HTL from 10 nm to 200 nm, it is found that the PCE and J_{SC} attain their maximum at 60 nm and then decreases when the thickness is increased.

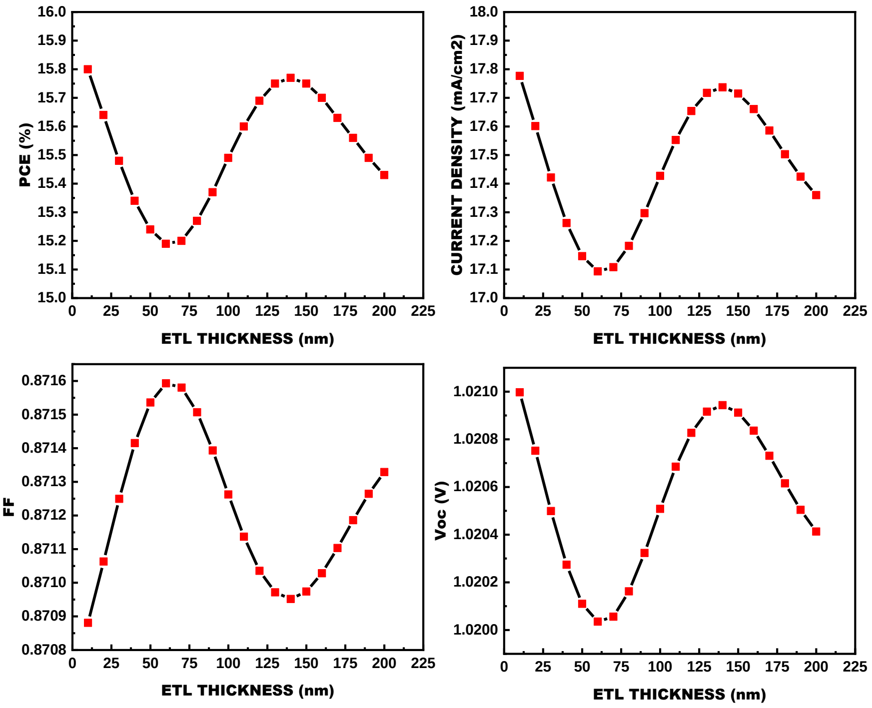

FIGURE 3. Shows how the PSC's efficiency varies as the ETL thickness increases.

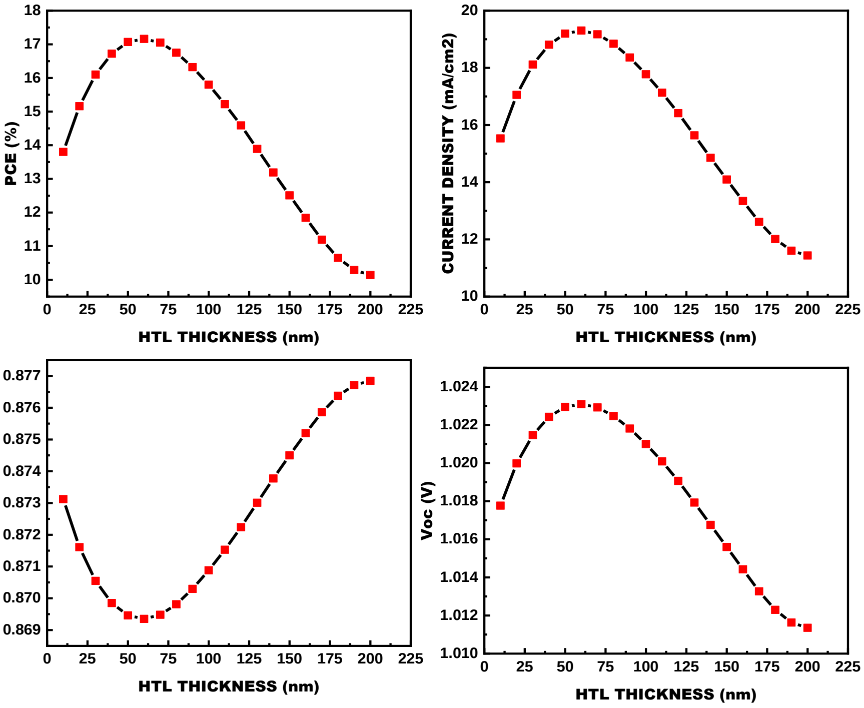

FIGURE 4. Shows how the PSC's efficiency varies as the HTL thickness increases

TABLE 2: shows the comparison among previously published reported and current work.

PSC DEVICE STRUCTURE	**PCE (%)**	**J_{SC} (mA/cm^2)**	**FF (%)**	**V_{OC} (V)**	**REFERENCES**
$FTO/TiO_2/CsSnI_3/Cu_2O/Au$	26.84	29.91	83.59	1.07	Our work
front contact/PCBM/ $CsSnI_3$/back contact	21.47	26.32	86.43	0.944	[4]
$FTO/TiO_2/CsSnI_3/P3HT/Au$	26.40	34.70	78.21	0.972	[1]
$SnO_2/CsSnI_3$/Spiro-OMeTAD	19.92	30.68	73.36	0.829	[3]
$ITO/PCBM/CsSnI_3/CFTS/Se$	24.73	33.99	83.46	0.872	[2]
$FTO/TiO_2/CsSnI_3/CZTSe/Au$	21.63	34.38	76.43	0.83	[5]
$FTO/ZnMgO/CsSnI_3/GO/Au$	17.37	35.61	78.21	0.624	[7]

TABLE 3: shows the Electrical IV key figures of the PSC.

PSC STRUCTURE	PCE (%)	J_{SC} (mA/cm^2)	FF (%)	V_{OC} (V)	EQE (%)
FTO/TiO_2/$CsSnI_3$/Cu_2O/Au	26.84	29.91	83.59	1.07	85.71

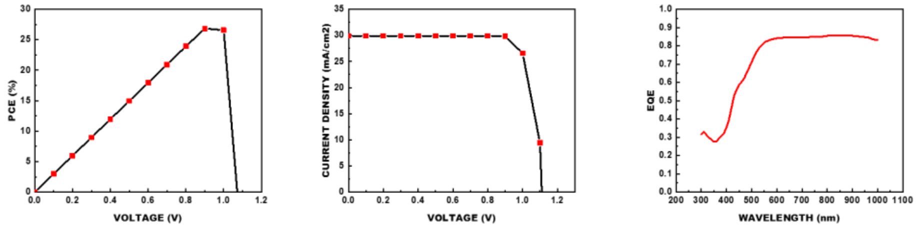

FIGURE 5. Shows the PSC performances A) PCE, B) J_{SC}, and C) EQE.

4 CONCLUSION

This study proposes a possible configuration: FTO/TiO_2/$CsSnI_3$/Cu_2O/Au. The highest possible power conversion efficiency can be achieved by optimizing the work functions of the electrodes, ETL, HTL, and perovskite layer thickness. When operating in the 300–1000 nm wavelength range and at 300 K, the PSC's PCE is 26.84%. When we compared our simulation work with other published work our proposed structure shows 0.44% greater PCE than the simulation found in the literature using the same Perovskite Absorber Layer.

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