Numerical Assessment of Highly Efficient Tin-Halide Perovskite Solar Cell

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Abstract. Interface science of Perovskite Solar cells (PSCs) has a very crucial role in increasing the efficiency of solar cells. The process of numerical simulation has also helped the solar cell’s efficiency to grow rapidly from 3.8% in 2009 to around 11% in 2010 in such a short period. This was a great achievement at that time and from then it kept on improving. Not only its rapid increase in efficiency attracted the researchers but also its low manufacturing cost and high $V_{oc}$. In this work, we will discuss the Lead-Free Perovskite Solar Cell (PSC) due to its non-toxic nature. A lot of research has already been done on Perovskite Solar Cell that has led to an increase in its efficiency. Despite the truth that they are toxic and can harm us anyway. The prime motive of producing electricity by using solar cells is to provide a cleaner way to produce electricity but if we are using toxic materials in the manufacturing of the cell, we are getting diverted. That’s why this research paper will focus on the cell having Sn in its absorber layer. The model we are discussing here will have $\text{CH}_3\text{NH}_3\text{SnI}_3$ (Absorber) as the Perovskite Layer which is non-toxic also the following different layers were also used in simulating our device such as ITO (Indium Tin Oxide) as the front contact, $\text{ZnO}$ (Zinc Oxide) as electron transporting layer (ETL), $\text{CuI}$ is acting as Hole transport layer (HTL) and we are using Gold (Au) as a back contact. The motive of this research is to make it non-toxic that we have already achieved and to make it highly efficient and the efficiency of the proposed device is 24.72%.

1. Introduction
With the increasing modernization in this world, humans are tending to be more dependent on machines, and hence more energy resource are required to satisfy our needs. There are many ways to produce electricity some of them being non-renewable and some being renewable sources but since the past few years, there is a lot of focus on renewable sources because they will not emit harmful gases and harmful by-products [3]. Solar energy is a very famous renewable source of energy and being recently mostly discussed it has now many advancements that are making it successful. The rapid increase in efficiency in such a short span of time is also appreciable [4]. Since the advent of solar energy, the solar industry has seen many types of devices and the recent popular one is Perovskite Solar Cells (PSCs)[2, 8, 11, 16, 17]. Photovoltaic cells can directly transform the rays we get from the sun into electricity [6].

The discussion of a perovskite solar cell is done here in this paper. The Perovskite solar cell has played a pivotal role in the solar industry due to its low costing, high efficiency, and high $V_{oc}$. Lead-
Halide Perovskite solar cells are quite famous but the lead in them makes us shift to its alternative that is the Tin-Halide Perovskite Solar Cell [5, 12, 17]. So, in this proposed device we will use CH$_3$NH$_3$SnI$_3$ instead of CH$_3$NH$_3$PbI$_3$. The Tin-Halide Perovskite layer is not only non-toxic but also has many other benefits such as a small band gap that is of 1.3eV and high absorption coefficient (α)[13]. We successfully attained a highly efficient device because of the combination of layers used and also their properties. Figure 1. shown below depicts the necessary layers of the solar cell we will use in this device.

In this work Tin-Halide, PSC will have the following five layers as Indium Tin Oxide/ Zinc Oxide/ Tin-Iodide Perovskite/ Copper Iodide/ Gold. In this proposed device ITO [7] is the front contact and sunlight will enter from here, the second layer is of ZnO which is the electron transport layer (ETL)[9], CH$_3$NH$_3$SnI$_3$ is a perovskite layer that behaves as an absorber, CuI and it is serving the purpose of the hole transport layer (HTL) and the role of back contact is fulfilled by Gold. A comparison is also done here with the other devices which will help us to assess our work.

2. Methodology and Simulation
The numerical simulation done here is done on Silvaco Technology CAD (Silvaco TCAD). The three-dimensional device structure and the meshing of the solar cell obtained are shown in Figure 2(a) and Figure 2(b). All the layers are clearly visible and then a discussion will be done on the functions and the properties of all the materials used.
The simulated device that is presented in this paper has the following layers- Indium Tin Oxide (ITO) this layer is 0.500 µm thick and it acts as a passage for sunlight to enter the device it is the widest layer of this device so that maximum sunlight can enter the device. This layer is also known as front contact. The second layer is Zinc Oxide (ZnO), this layer serves as the electron transport layer (ETL) and its primary objective is to throw back holes towards HTL, this layer is 0.080 µm thick. The next layer is the Perovskite layer and which is 0.350 µm thick and is also known as the absorber layer. The material used in the next layer is CuI and it is serving as the hole transport layer. The final layer is of gold and it is 0.020 µm thick and it serves the purpose of back contact in this device. All the materials along with their electrical properties are shown in Table 1. given below.

Table 1. Parameters used in the simulation of Tin-Halide PSC.

| Material | Thickness | Dopin g Type | Permittivi ty ε ε (relative) | Band Gap (eV) | χ (eV) | μn (cm²/V/s) | μp (cm²/V/s) |
|----------|-----------|--------------|-----------------------------|--------------|--------|--------------|--------------|
| x-axis (µm) | y-axis (µm) | z-axis (µm) | | | | | |
| ITO | 10 | 0.500 | - | - | - | - | - |
| ZnO | 10 | 0.080 | - | 8.12 [1] | 3.2 [15] | 4.29 [1] | 200 | 5 |
| Perovskite | 10 | 0.350 | - | 8.2 [18] | 1.3 [18] | 4.17 | 1.6 | 1.6 |
| CuI | 10 | 0.100 | - | 10 [19] | 3.2 [19] | 4.1 [19] | 1.69e-4 | 1.69e-4 |
| Gold | 10 | 0.020 | - | - | - | - | - |

3. Results and Discussions

![Figure 3. Comparison of different Solar Cells.](image)
After simulating our device, the value of the following parameters was obtained $J_{sc}$, $V_{oc}$, FF, and efficiency. A comparison is also done with a device that had CH$_3$NH$_3$PbI$_3$ as the absorber layer instead of CH$_3$NH$_3$SnI$_3$ and also with a device having a different Electron Transport Layer (ETL). The comparison is also shown graphically. The graph is represented in Figure 3. Through this bar graph, it can be noticed that the parameters such as open-circuit voltage($V_{oc}$), Fill Factor (%), and efficiency shoot up. Through the bar graph shown above, we can clearly interpret that the efficiency of the solar cell has been increased significantly and the combination of layers used is successfully increasing its efficiency. There is very little difference in the value of $V_{oc}$ but still, the open-circuit voltage of the proposed device is better as compared to the other two devices and it is helping efficiency to increase[10]. The Value of the Fill Factor is also maximum in the device proposed having layers (ZnO/CH$_3$NH$_3$SnI$_3$/CuI) as compared to the other two. Optimization of thickness and other properties made it possible to achieve an efficiency of 24.72%. Values of various parameters calculated are shown in Table 2.

| Parameters | Values |
|------------|--------|
| $J_{sc}$ (mA/cm$^2$) | 24.2 |
| $V_{oc}$ (V) | 1.06 |
| FF (%) | 81.8 |
| Eff (%) | 24.72 |

The architecture of Tin-Halide PSCs has exceptional features such as non-toxic, low-cost easy fabrication. The numerical simulation of the device helped us to observe the effect of different materials very easily and it also helps in the investigation of different attributes of different layers [14]. Many graphs are also obtained that verifies the credibility of this device. The graph of Wavelength vs Photon energy simulated by running it on Silvaco TCAD is clearly shown in Figure 4. and it can be clearly interpreted that upon decreasing wavelength of rays the potential starts to increase and then after a point that is around 1000 nm and the maximum potential obtained is 1.06 V. The potential started decreasing gradually. It is also verified theoretically as the wavelength is inversely proportional to the square root of potential.

![Figure 4. Wavelength as a function of photon energy.](image)
The graph of specific capacitance vs potential is represented in the curve given in Figure 5. With the increasing potential, the value of capacitance is increasing and it is interpreted from it that the maximum capacitance is obtained at around 0.75 V and the capacitance obtained is about 158 nF/cm². Also, a curve between absorption constant i.e. $\alpha$ and optical wavelength is shown below in Figure 6. represents three different layers that are CuI, Perovskite, and ZnO through this curve we can interpret that the absorption constant of different layers is best in the range of 300nm to 900 nm and it is decreasing gradually with the increasing value of wavelength that is why the wavelength of light used for illumination is set to be at 0.350 µm. The graphs here portray the penetration of the rays in the cell.

![Specific capacitance vs Potential](image)

**Figure 5.** Specific capacitance vs potential.

![Absorption constant vs Wavelength](image)

**Figure 6.** Absorption constant plots for CuI, Perovskite and ZnO with respect to wavelength.
The next curve is shown in Figure 7, represents the variation of current density w.r.t potential at different values of thickness of absorber layer that is perovskite. It helps us in understanding that somewhere in between 0.233 μm and 0.700 μm we found the value of potential to be maximum and hence the value of 0.350 μm was used in the simulation. The different thicknesses of perovskite used in the simulation to find the optimization value were done and the graph is shown in Figure 8. This figure is showing that is the quantum efficiency will be maximum somewhere between 0.233 μm and 0.700 μm and hence the value of 0.350 μm was used and the maximum efficiency obtained after simulating the whole device was found to be 24.72%.

![Current Density vs Potential](image1.png)

**Figure 7.** Current density vs potential.

![Quantum Efficiency vs Wavelength](image2.png)

**Figure 8.** Quantum efficiency (QE%) vs wavelength.
The contour plots are shown in Figure 9 (a) and (b) represents the total current density and recombination rate. It can be observed that the perovskite solar cell with CH$_3$NH$_3$SnI$_3$ as the absorber layer and CuI as Hole Transport Layer (HTL) has a very high current density and also the recombination taking place in the device is decreasing and it is clearly visible in the absorber region as we all know more the recombination in absorber region lesser will be its efficiency. Hence a highly efficient solar cell is formed. Similarly, the graphs of hole concentration and electric field of perovskite solar cells having CH$_3$NH$_3$SnI$_3$ as its absorber layer and CuI as HTL are shown in Figure 9 (c) and (d). The contour plot of hole concentration is also supporting the increased efficiency of our device. Electric Field shown below is showing a varying electric field in the Hole Transport Layer and that is how the efficiency of 24.72% was achieved.

![Figure 9. Contour plots of (a)Total Current Density, (b) Recombination rate, (c) Hole concentration, and (d) Electric Field of the proposed PSC.](image)

4. Conclusion
Numerical optimization of layers was done such as their doping concentration and thickness hence we got to observe that the thickness of the layer plays a crucial role in increasing the Power Conversion Efficiency (PCE). The efficiency of every solar cell depends mostly on the thickness of its absorber layer as not only the absorption of sunlight takes place but the electron-hole pairs are also generated here. On decreasing the thickness of the absorber, the recombination of charges will increase thus decreasing the absorption and then efficiency. The results shown by the proposed device are satisfying and the comparison done was also supporting the work presented here. Different electrical parameters such as current density, open-circuit voltage, Fill Factor, and Efficiency were calculated efficiency of 24.72% was obtained. Perovskite solar cells can be seen as a promising candidate for future research as well because there is a huge scope of improvement such as we can further work on increasing its stability and also on the materials which can be used as its back contact instead of gold as it is expensive.

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