Design and Modelling of Eco-Friendly CH$_3$NH$_3$SnI$_3$-Based Perovskite Solar Cells with Suitable Transport Layers

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Abstract: An ideal n-i-p perovskite solar cell employing a Pb free CH$_3$NH$_3$SnI$_3$ absorber layer was suggested and modelled. A comparative study for different electron transport materials has been performed for three devices keeping CuO hole transport material (HTL) constant. SCAPS-1D numerical simulator is used to quantify the effects of amphoteric defect based on CH$_3$NH$_3$SnI$_3$ absorber layer and the interface characteristics of both the electron transport layer (ETL) and hole transport layer (HTL). The study demonstrates that amphoteric defects in the absorber layer impact device performance significantly more than interface defects (IDL). The cell performed best at room temperature. Due to a reduction in $V_{oc}$, PCE decreases with temperature. Defect tolerance limit for IL1 is $10^{13}$ cm$^{-3}$, $10^{16}$ cm$^{-3}$ and $10^{12}$ cm$^{-3}$ for structures 1, 2 and 3 respectively. The defect tolerance limit for IL2 is $10^{14}$ cm$^{-3}$. With the proposed device structure FTO/PCBM/CH$_3$NH$_3$SnI$_3$/CuO shows the maximum efficiency of 25.45% ($V_{oc}$ = 0.97 V, $J_{sc}$ = 35.19 mA/cm$^2$, FF = 74.38%), for the structure FTO/TiO$_2$/CH$_3$NH$_3$SnI$_3$/CuO the best PCE is obtained 26.92% ($V_{oc}$ = 0.99 V, $J_{sc}$ = 36.81 mA/cm$^2$, FF = 73.80%) and device structure of FTO/WO$_3$/CH$_3$NH$_3$SnI$_3$/CuO gives the maximum efficiency 24.57% ($V_{oc}$ = 0.90 V, $J_{sc}$ = 36.73 mA/cm$^2$, FF = 74.93%) under optimum conditions. Compared to others, the FTO/TiO$_2$/CH$_3$NH$_3$SnI$_3$/CuO system provides better performance and better defect tolerance capacity.

Keywords: CH$_3$NH$_3$SnI$_3$; CuO; HTL; WO$_3$; perovskite; SCAPS-1D

1. Introduction

The usage of renewable energy, especially solar photovoltaic as an alternative to conventional power generation sources, has enormous potential to reduce global warming significantly. Among the different types of solar cells, third-generation perovskite solar cells are currently the centre of interest in the scientific community as they offer a new area for solar energy research and can be implemented at a low cost with great efficiency [1]. A typical
perovskite structure is denoted as ABX₃, where A is a monovalent cation (i.e., cesium ion, methylammonium ion, formamidine ion); B is a di-, tri-, or tetravalent metal ion (i.e., Pb²⁺, Sn²⁺, Ge²⁺, Sb³⁺, Bi³⁺ or Ti⁴⁺); and X is a halide anion (i.e., Cl⁻, Br⁻, I⁻) [2–8]. Despite the tremendous advantages of Pb-based perovskite, scientists around the world are trying to replace the toxic Pb with other non-toxic metallic ions without compromising the overall cell efficiency. In this regard, tin (Sn)-based perovskites are gaining popularity because of their suitable bandgap [9], excellent photovoltaic properties [10], cheap fabrication cost [11], excellent performance [12], and environmental friendliness [9]. Shockley–Queasier (SQ) limit is the maximum efficiency limit that converts sunlight into electric energy. Considering a single p-n junction with a 1.4 eV band gap, the highest solar conversion efficiency is calculated 32.91 [13]. Till now, the record 25.6% power conversion efficiency has been achieved for FAPbI₃ using pseudo-anion engineering during the fabrication process [14]. It is already reported that surface passivation, structural and interface engineering can improve the stability of the cell [15,16]. Again, the performance of Sn-based PSCs lags compared to Pb-based PSCs because of the oxidative nature of divalent Sn [10,17]. Moreover, defect free crystallization of Sn-based perovskite significantly impacts cell performance. Though several efforts have been made to tackle the aforementioned issues and prevent the occurrence of defects [18–28], there is still ample room for improvement as the maximum efficiency (13.24%) for SnX₃-based perovskite solar cells (PSCs) [29] and stability reached at 3800 h [30] are still lower than its SQ limit.

Hence, in this article we model different types of electron transport materials for SnX₃-based perovskite solar cells for achieving higher efficiency. In this regard, three different device structures have been considered: FTO/PCBM/CH₃NH₂SnI₃/CuO/back metal (Structure 1), FTO/TiO₂/CH₃NH₂SnI₃/CuO/Back metal (Structure 2) and FTO/WO₃/CH₃NH₂SnI₃/CuO Back metal (Structure 3). An electron transport layer (ETL) composed of TiO₂ in PCSs can enhance the capture and transportation of electrons that reduce the recombination losses of solar cells [31]. PCBM is used as ETL material due to its easy fabrication, low hysteresis effect and excellent device performance [32,33]. WO₃ showed comparable optical characteristics to TiO₂, but it has a greater electrical conductivity [34], low hysteresis effect [35], is printable, stable and a low annealing temperature is required during the fabrication process [36]. CuO was chosen as the hole transport layer (HTL) because of its superior charge accumulation characteristics, high hole mobility, availability, band alignment perfectly match with CH₃NH₂SnI₃, solution processability and excellent chemical stability [37]. The main goal of this simulation is to compare the effect of defects density of different ETL materials for SnX₃-based perovskite solar cells. PCMB, TiO₂, and WO₃ have been described as ETLs for SnX₃-based perovskite solar cells in the literature [38–44]. Besides this, there are a limited number of reports on CuO as HTL [45,46]. Researchers could better comprehend SnX₃-based perovskite solar cells’ performance with different ETL and CuO HTL by comparing them. In addition, temperature effects, amphoteric defect state in CH₃NH₂SnI₃ absorber layer, analyzing both of its interface’s properties with defect concentration, the effect of back contact metals, Mott-Schottky analysis and the effect of series resistances are all carefully investigated to understand their impact on cell performance and achieve enhanced power conversion efficiency (PCE).

2. Materials and Methods

In this work, a n-i-p structure is proposed and Sn-based perovskite is employed as an absorber. As a result, solar radiation will penetrate to the electron transport layer. A standard spectrum of AM1.5G (1000 W/m²; T = 300 K) has been used for the illumination. The thickness was kept fixed for all simulation results. Initially, the thickness of the absorber layer was first optimized using simulation, and the thickness of the remaining layers was determined based on the literature. The ideal SnX₃-based perovskite structure is shown in Figure 1. To examine the effect of defect densities, except interface defect concentration change, overall defect density was maintained constant at 10¹⁰ cm⁻³ for ETL/perovskite and perovskite/HTL interfaces. During simulation, the thermal velocity of electrons and
holes was defined to be $1 \times 10^7$ cm/s. A number of articles support all the criteria used in this analysis [4,47–61]. Table 1 shows the simulation parameters used in this article.

The device configuration of the simulated FTO/PCBM/$\text{CH}_3\text{NH}_3\text{SnI}_3$/CuO/Back metal (Structure 1), FTO/TiO$_2$/CH$_3$NH$_3$SnI$_3$/CuO/Back metal (Structure 2), FTO/WO$_3$/CH$_3$NH$_3$SnI$_3$/CuO Back metal (Structure 3) solar cells and the corresponding band diagrams are shown in Figure 2a–c.

![Figure 1. Building Block of $\alpha$-CH$_3$NH$_3$SnI$_3$ [47] (COD Id = 4335632), Color code: I = Blue, Sn = Yellow, C = Red, N = Purple.](image)

![Figure 2. Schematic diagram of proposed perovskite solar cell’s structure and Energy band alignment; (a) Structure 1, (b) Structure 2 and (c) Structure 3.](image)
Table 1. Simulation parameters for perovskite solar cell using SCAPS-1D.

| Parameters                             | PCBM  | WO$_3$ | TiO$_2$ | CH$_3$NH$_3$SnI$_3$ | CuO  |
|----------------------------------------|-------|--------|---------|---------------------|------|
| Thickness (nm)                         | 50    | 50     | 50      | 700                 | 50   |
| Bandgap (eV)                           | 2 [48] | 2.92 [49] | 3.2 [37,41] | 1.23 [42,43] | 1.48 [53] |
| Electron affinity (eV)                 | 4.2 [40] | 4.59 [54] | 4.1 [4] | 4.17 [4,42] | 4.07 [56] |
| Dielectric permittivity (relative)     | 3.9 [40] | 5.76 [54] | 9 [44,45] | 10 [40,46] | 18.1 [56] |
| CB effective density of states (1/cm$^3$) | $2.5 \times 10^{21}$ [40] | $1.96 \times 10^{19}$ [54] | $2.2 \times 10^{18}$ [4] | $1 \times 10^{19}$ [40] | $2.1 \times 10^{19}$ [56] |
| VB effective density of states (1/cm$^3$) | $2.5 \times 10^{21}$ [40] | $1.96 \times 10^{19}$ [54] | $1 \times 10^{19}$ [40] | $1 \times 10^{19}$ [40] | $5.5 \times 10^{19}$ [60] |
| Electron thermal velocity (cm/s)       | $1 \times 10^7$ [40] | $1 \times 10^7$ [54] | $1 \times 10^7$ [61] | $1 \times 10^7$ [59] | $1 \times 10^7$ [59] |
| Hole thermal velocity (cm/s)           | $1 \times 10^7$ [40] | $1 \times 10^7$ [54] | $1 \times 10^7$ [61] | $1 \times 10^7$ [59] | $1 \times 10^7$ [59] |
| Electron mobility (cm$^2$/Vs)          | 0.2 [40] | 10 [54] | 20 [57] | 1.6 [40,42,49] | 0 [56] |
| Hole mobility (cm$^2$/Vs)              | 0.2 [40] | 10 [54] | 10 [57] | 1.6 [40,42,49] | 0.1 [56] |
| Shallow uniform acceptor density, NA (1/cm$^3$) | 0 | 0 | 0 | $3 \times 10^{17}$ [40] | $1 \times 10^{16}$ [56] |
| Shallow uniform donor density, ND (1/cm$^3$) | $2.93 \times 10^{17}$ [40] | $3.68 \times 10^{19}$ [54] | $1 \times 10^{18}$ [58] | $3 \times 10^{17}$ [40] | 0 |
| N$_t$ total (1/cm$^3$)                 | $1 \times 10^{14}$ | $1 \times 10^{14}$ | $1 \times 10^{14}$ | $1 \times 10^{14}$ | $1 \times 10^{14}$ |

3. Results

3.1. Effect of Amphoteric Defect Density in the Absorber Layer

The impact of native imperfections on semiconductors is referred to as an “amphoteric defect” [62]. The fundamental characteristic of this type of defect is the Fermi level stabilization energy (EFS) [63]. Even though in balanced growth conditions for any thin film, native faults are natural components that are practically intrinsic in crystal structures [64], these defects produce short minority carrier lifetimes, resulting in lower $V_{oc}$ in solar cells [65].

The thickness of the absorber layer is considered 0.7 µm, as established by a prior study [66]. Figure 3 shows the impact of amphoteric defects on the absorber layer when defect concentration is raised from $10^{11}$ cm$^{-3}$ to $10^{16}$ cm$^{-3}$. We noticed that $V_{oc}$ and $J_{sc}$ are virtually identical up to the defect concentration of $10^{15}$ cm$^{-3}$. When the defect concentration is boosted from $10^{15}$ cm$^{-3}$ to $10^{16}$ cm$^{-3}$, $V_{oc}$, $J_{sc}$ and FF decrease drastically. For the device structures 1 (Figure 2a) and 2 (Figure 2b), the $V_{oc}$ reduced from approximately 0.8 V to about 0.7 V (Figure 3a,b) and $V_{oc}$ dropped from 0.89 V to about 0.69 V for Structure 3 (Figure 3c) at $10^{16}$ cm$^{-3}$ defect density. Figure 3d illustrates the impact of defect density on $J_{sc}$ and FF for three different ETLs on SnX$_3$-based perovskite structures. $J_{sc}$ decreased from 35.02 mA/cm$^2$ to 27.49 mA/cm$^2$, 36.71 mA/cm$^2$ to 30.76 mA/cm$^2$, 36.71 mA/cm$^2$ to 22.91 mA/cm$^2$ for structures 1, 2 and 3, respectively. FF is decreased from 76.12% to 59.45%, 78.57% to 61.98% and 73.23% to 59.23% for structures 1, 2 and 3, respectively.

With the defect concentration from $10^{15}$ cm$^{-3}$ to $10^{16}$ cm$^{-3}$, PCE is decreased 21.32% to 11.37%, 23.61% to 13.51% and 23.97% to 7.74% for the structures 1, 2 and 3, respectively. The negative impact on solar cell performance may be due to the greater recombination rates and shorter diffusion times for photogenerated charge carriers derived from higher defect densities, so in each case, the defect tolerance limit for the proposed structures is considered $10^{15}$ cm$^{-3}$.
3.2. Effect of Interfacial Defect Density ETL/CH$_3$NH$_3$SnI$_3$ (IL1) and CH$_3$NH$_3$SnI$_3$/CuO (IL2)

To improve cell efficiency, recombination loss at interfaces should be reduced [67]. Recently, considerable approaches have been described for interface remodelling to avoid recombination [68–71]. In this simulation defect states were investigated in both interface layers ETL/CH$_3$NH$_3$SnI$_3$ and CH$_3$NH$_3$SnI$_3$/CuO.

For IL1, single energetic distribution has been considered. Figure 4b shows that with the IL1 defect condition for device 2, virtually there is no significant changes occurred on the cell performance. $V_{oc}$ is almost constant up to the defect density of $10^{16}$ cm$^{-3}$. Moreover, it is seen that when defect density rises from $10^{11}$ cm$^{-3}$ to $10^{17}$ cm$^{-3}$, $V_{oc}$ drops continuously from 0.97 V to 0.7 V and 0.85 V to 0.57 V for structures 1 and 3, respectively (Figure 4a,c). As seen in Figure 4d, with the increasing defect concentration up to $10^{15}$ cm$^{-3}$ no significant changes occurred for $J_{sc}$ for all structures. Above this concentration $J_{sc}$ drastically decrease for structures 1 and 3. For device 2, no significant changes occurred on FF up to defect density of $10^{16}$ cm$^{-3}$ but above this density a marginal increase of FF is observed. FF is decreased drastically for structures 1 and 3 above the defect concentration of $10^{14}$ cm$^{-3}$. PCE remains almost constant for structure 2. But PCE decreased significantly from the defect density of $1 \times 10^{13}$ cm$^{-3}$ and $1 \times 10^{12}$ cm$^{-3}$ for structures 1 and 3, respectively. PCE is decreased mainly due to the decrement of $V_{oc}$. So, IL1 defect tolerance limit of structure 1 is $1 \times 10^{13}$ cm$^{-3}$ and structure 3 is $1 \times 10^{12}$ cm$^{-3}$. Low defect tolerance limit may be due to extensive carrier recombination at the interface and lower the device performance [72]. A defect tolerance limit may be predicted at interface TiO$_2$/CH$_3$NH$_3$SnI$_3$ for structure 2 is $1 \times 10^{16}$ cm$^{-3}$. The high defect tolerance limit of the device indicates a well-matched conduction band offset between TiO$_2$ and perovskite, which creates an effective interfacial electric field that prompts carrier extraction, resulting in improved cell stability and performance [73]. The higher defect tolerance limit at the interface, making it more appropriate for fabrication.
As seen from Figure 5a, cell efficiency has dropped when the defect density at IL2 raised to $1 \times 10^{14}$ cm$^{-3}$ or higher, from 25.39% to 23.14%, 26.85% to 24.56% and 24.63% to 21.62% for structures 1, 2 and 3, respectively. With increasing defect density $V_{oc}$ drops from around 0.99 V to 0.80 V for structures 1 and 2 (Figure 5a,b). For device 3, $V_{oc}$ drops from about 0.99 V to 0.80 V (Figure 5c). Above a defect density of $1 \times 10^{14}$ cm$^{-3}$, a drastic decrement of $V_{oc}$ is observed in all cases. The recombination rate increases as the defect density state at the interface rise, causing the reverse saturation current to increase and the open-circuit voltage to drop. PCE is decreased mainly due to the decrement of $V_{oc}$. The relationship between $J_{sc}$, FF, PCE, and defect states in the CH$_3$NH$_3$SnI$_3$/CuO interface is shown in Figure 5d. There are no significant changes that occurred for $J_{sc}$ with increasing the defect density for all three proposed structures. Above the defect density of $10^{14}$ cm$^{-3}$, FF is increased for structures 1 and 2, but a negligible decrement is observed for structure 3.

The ideality factor ($n$), which is linked to the nature of the semiconductor, influences carrier generation, its transportation at the interface and collection at the terminal contact. An increase in the ideality factor has a direct and negative effect on the fill factor of solar cells [74]. For structures 1 and 2, the FF increment indicates a low ideality factor and a reduction in reverse saturation current above a defect density of $10^{14}$ cm$^{-3}$. Variations in the amount of defect state have been shown to have a greater influence on $V_{oc}$ than $J_{sc}$. As a result, changes in $V_{oc}$ are primarily responsible for the device’s decreased efficiency. Consequently, the CH$_3$NH$_3$SnI$_3$/CuO interface defect tolerance is considered $10^{14}$ cm$^{-3}$, as the efficiency of each device falls considerably over that limit.
The effect of various metals as back contact electrodes on the performance of PSCs has been investigated as represented in Table 2.

Table 2. Metal work function of back contact material.

| Back Contact Metals | Cu    | C     | Ni    | Au    |
|---------------------|-------|-------|-------|-------|
| Work Function (eV)  | 4.9 [75] | 5 [76] | 5.15 [77] | 5.3 [78] |

Simulations have been done using copper (Cu), carbon (C), nickel (Ni) and gold (Au) as prospective back contacts for perovskite solar cells. An Ohmic contact between ETL and electrode is required for the smooth collection of electrons to the load [79]. A relatively high work function is appropriate for back contact materials. From Figure 6, it is seen that with increasing work function of back contact materials, the efficiency of perovskite solar cells increases. It is found that Au as a back electrode material indicates the highest efficiency of 24.58% for device 1, 26.02% for device 2 and 23.53% for device 3. In comparison best performance of the cell is obtained when TiO₂ is used as ETL material in device 2.

3.3. Metal Work Function

The amount of energy or photons required to remove an electron from a metal’s surface is known as its work function. It has been found that a larger work function value increases solar cell efficiency. This is due to the fact that when the work function value increases, the majority carrier’s barrier height drops, making contact more ohmic in nature. The effect of various metals as back contact electrodes on the performance of PSCs has been investigated as represented in Table 2.

Figure 5. Effect of interfacial defect concentration (N_t) at IL2 interface; PCE and V oc vs. interfacial defect concentration for (a) Structure 1, (b) Structure 2 and (c) Structure 3, (d) J sc, FF and efficiency vs. interfacial defect concentration in IL2.
A built-in potential ($V_{bi}$) is required to move photogenerated holes and electrons in opposing directions [80]. The junction potential difference in a solar cell generates $V_{bi}$. High built-in potential is required to prevent significant losses due to carrier recombination processes in solar cells in order to ensure effective energy conversion. In this work, Schottky contact is formed in ETL/Front contact. $V_{bi}$ can be obtained from a Mott-Schottky capacitance study. A space charge effect is responsible for the rise in capacitance. When the voltage rises, the depletion width narrows, resulting in an increase in capacitance. Following a particular voltage drive, the capacitance is again declined and can even be negative. Recombination or self-heating can generate negative capacitances as well [81]. Mott-Schottky analysis is a prominent method to obtain doping concentration and the built-in voltage which is expressed by the following relationship:

$$\frac{1}{C^2} = \frac{2}{S \cdot \varepsilon \cdot q} \cdot \frac{1}{N_A} \cdot (V_{bi} - V)$$

(1)

where $C = $ capacitance, $S = $ area, $\varepsilon = $ vacuum permittivity, $N_A = $ dopant density and $V_{bi} = $ built-in voltage. Figure 7X,Y show that the C-V and Mott-Schottky plot and simulation features, respectively, as a function of ETL’s shallow uniform donor density ($N_d$) for three simulated devices (Figure 7a–c). A simulation was done for donor density ($N_d$), where concentration was ranged from $10^{16}$ cm$^{-3}$ to $10^{20}$ cm$^{-3}$, keeping other factors as constant. We know that carrier recombination solely takes place at the donor-acceptor interface where $V_{oc}$ does not affect the built-in voltage. On the other hand, the fill factor (FF) is significantly lowered when the built-in voltage drops below the open-circuit voltage [82]. In this study, it has been found that with the voltage applied, capacitance increases gradually and rises sharply when the $N_d$ is $10^{20}$ cm$^{-3}$. The $V_{bi}$ is obtained from the voltage axis intersect. The built-in potential ($V_{bi}$) has been found to increase from 0.71 V to 0.78 V with the increase of $N_d$ for structures 1 and 2 (Figure 7Ya,b)), but for Structure 3, it is ranged from 0.44 to 0.65 V (Figure 7Yc)). This means that a greater carrier recombination rate reduces the $V_{bi}$ value in structure 3. High built-in potential for structures 1 and 2 denotes the rapid movement of the photogenerated holes and electrons in opposing directions makes the devices for a better choice of fabrication.

Figure 6. Solar cell efficiency for different back contact metals.

3.4. C-V Characteristics of the Cell

In this study, it has been found that with the voltage applied, capacitance increases gradually and rises sharply when the $N_d$ is $10^{20}$ cm$^{-3}$. The $V_{bi}$ is obtained from the voltage axis intersect. The built-in potential ($V_{bi}$) has been found to increase from 0.71 V to 0.78 V with the increase of $N_d$ for structures 1 and 2 (Figure 7Ya,b)), but for Structure 3, it is ranged from 0.44 to 0.65 V (Figure 7Yc)). This means that a greater carrier recombination rate reduces the $V_{bi}$ value in structure 3. High built-in potential for structures 1 and 2 denotes the rapid movement of the photogenerated holes and electrons in opposing directions makes the devices for a better choice of fabrication.
3.5. Effect of Series Resistance

The performance of perovskite solar cells is limited due to the series resistance of the device. In an ideal solar cell, series resistance ($R_s$) will be zero and shunt resistance ($R_{SH}$) should be infinitive [83]. The transparent conductive oxide layer is one of the primary contributors to the series resistance ($R_s$) [84]. $R_s$ is derived from current flow resistance in PSCs, in particular through interfaces [72]. The FF of the device is influenced by its $R_s$ and $R_{SH}$ [85]. Excessive series resistance values ($R_s$) can also lower the $J_{sc}$. The relationship of output current and the series resistance is given below:

$$I = I_L - I_0 \exp \left[ \frac{q(V + IR_s)}{nkT} \right] - \frac{V + IR_s}{R_{SH}}$$  

(2)

Here, $I = \text{output current}$, $I_L = \text{light generated current}$, $R_{SH} = \text{shunt resistance}$ and $R_s = \text{series resistance}$, $q$ and $k$ are constants, $T = \text{absolute temperature}$. The FF and PCE with series resistances ($R_s$) on the proposed CH$_3$NH$_3$SnI$_3$ based three solar cell structures are shown in Figure 8. It has been found that increasing series resistance has a negative impact mostly on the FF due to solder bond degradation [86].

The solder bond undergoes fatigue or cracks in an open environment that leads to increasing series resistance. The series resistance correlates to a drop in fill factor (FF) as follows [87]:

$$\Delta \text{FF} = -(J_{sc}/V_{oc}) \times R_{s(\text{total})} \times \text{FF}_{\text{ideal}}$$  

(3)

Once $R_s$ is unusually high, it has a little observed impact on the $J_{sc}$. Figure 8 shows that above $R_s = 3 \text{ ohm-cm}^2$, FF degrades dramatically for structures 2 and 3. That’s because the interface solder bonding may not be strong enough at a higher $R_s$ value. Due to relatively strong interface solder bonding for structure 1, the rate of efficiency and FF degradation is virtually constant. The FF degradation rate of solar cells is about $3.4 \pm 0.2\%$ per 1 $\Omega$ rise in $R_s$, which is much lower than that of typical Si solar cells (roughly 2.5 percent for 0.1 increase in $R_s$). The FF of the Si solar cell reduces by about 2.5% each time the series
resistance increases by 0.1 Ω [88]. However, whereas FF declines at 3.4 ± 0.2%, efficiency only decreases at 1.15 ± 0.1% with a 1 rise in Rs. The proposed solar cell structures are much better than the conventional Si solar cell in terms of series resistance.

![Figure 8](image-url)  
*Figure 8.* The rate of change of FF and PCE with respect to series resistances (Rs).

### 3.6. Effect of Temperature

Working temperatures significantly influence perovskite solar cell performance, as they are placed in an open environment. The effect of temperature has been investigated from 300 K to 400 K, and the result shows that cell performance is greatly influenced by temperature, as seen in Figure 9. Cell efficiency is lowered with temperature rises because photovoltaic parameters (i.e., bandgap, electron and hole mobility, and carrier concentration) are influenced by higher temperatures [89]. The following equation is used to determine the open-circuit voltage (Voc) of a solar cell [90]:

$$V_{oc} = \frac{nKT}{q} \ln\left(\frac{J_{sc}}{J_0} + 1\right)$$  (4)

where, $K = $ Boltzmann constant, $T = $ absolute temperature in Kelvin and $J_0 = $ reverse saturation current. According to Equation (1), a low reverse saturation current is necessary to increase $V_{oc}$. Reverse saturation current is responsible for the decrement of $V_{oc}$ as temperature rises. The hypothesis might be that the peripheral increase of $J_{sc}$ with temperature that the bandgap in the semiconductor will be reduced with the increasing temperature [91]. Interatomic spacing of atoms of semiconductors increases with temperature hence decrease the band gap. In general, when temperature rises, electrical mobility and conductivity increases [92]. As seen from Figure 9, there is no significant change of $J_{sc}$ with temperature for structures 1 and 2. A decrease in $J_{sc}$ with high temperature has occurred for Structure 3 might be due to the fact the electrons are unstable at high temperature and recombine with the holes [93]. Lattice scattering is the primary process that influences electron and hole mobility as frequency scattering rises with temperature, so at high temperatures the carrier mobility should decrease, and the resistivity will increase.

As observed from Figure 10, the efficiency of the proposed three perovskite solar cells with PCBM, TiO$_2$, and WO$_x$ ETLs decreases as the temperature rises. For Structure 1, the efficiency is decreased at around 0.058%/K, but at higher temperature (400 K) the value is 0.15%/K. In case of Structure 2 the degradation gradient is almost constant at the value of 0.064 a.u. The degradation gradient decreases exponentially with temperature for structure 3 but the value is lower than that of structures 1 and 2 makes it more thermal stable. At higher temperature structures 2 and 3 provide more thermal stability than Structure 1. The low value of the degradation gradient indicates the possibility of real device fabrication for all the proposed three structures.
The efficiency with temperature is decreased. It is suggested to install the devices with a cooling water system to reduce the carrier’s thermal scattering and heating effect. With an amphoteric defect density of more than $10^{15}$ cm$^{-3}$, the device performance was greatly reduced. Interfaces defect tolerance limit for IL1 is $10^{13}$ cm$^{-3}$, $10^{16}$ cm$^{-3}$, $10^{12}$ cm$^{-3}$ for structures 1, 2, and 3.

### Figure 9. Effect of temperature on cell performance.

![Figure 9](image1.png)

### Figure 10. Degradation gradient of PSC for different electron transport layers.

![Figure 10](image2.png)

### 4. Conclusions

In this work, SCAPS software was utilized to conduct a comprehensive simulation analysis on the lead-free CH$_3$NH$_3$SnI$_3$ perovskite materials featuring superior optoelectronic characteristics and environmental effects. The numerical simulation is mostly concerned with temperature, amphoteric defects of the absorber layer, and defect study of the interfaces. A comparative study of three devices was performed. In every case the device works best at room temperature. It is suggested to install the devices with a cooling water system to reduce the carrier’s thermal scattering and heating effect. With an amphoteric defect density of more than $10^{15}$ cm$^{-3}$ the device performance was greatly reduced. Interfaces defect tolerance limit for IL1 is $10^{13}$ cm$^{-3}$, $10^{16}$ cm$^{-3}$, $10^{12}$ cm$^{-3}$ for structures 1,
2 and 3 respectively. Interfaces defect tolerance limit for IL2 was found 10^{14} \text{cm}^{-3}. The device structure of FTO/TiO_2/CH_3NH_3SnI_3/CuO/back electrode exhibits a better defect tolerance limit. It is found that the use of Au as a back-contact material provides the highest efficiencies of 25.45%, 26.92% and 24.73% for structures 1, 2 and 3, respectively. This simulation shows that eco-friendly CH_3NH_3SnI_3 can be used as a high-efficiency photovoltaic device.

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**List of Abbreviation**

| Abbreviation | Meaning |
|--------------|---------|
| ETL          | Electron transport layer |
| HTL          | Hole transport layer |
| PCE          | Power conversion efficiency |
| J_{sc}       | Short circuit current |
| V_{oc}       | Open circuit voltage |
| J_0          | Reverse saturation current |
| FF           | Fill factor |
| FTO          | Fluorine doped tin oxide |
| IL           | Interface defect layer |
| IL           | Interface layer |
| COD          | Crystallography Open Database |

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