Research Article

A Numerical Approach to Analysis of an Environment-Friendly Sn-Based Perovskite Solar Cell with SnO2 Buffer Layer Using SCAPS-1D

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1. Introduction

Energy usage is expected to increase significantly in the future. Most energy utilized today comes from fossil fuels, which have a large carbon footprint and will decay quickly. As a result of industrialization and population increase, energy prices are growing. The most challenging task is developing a renewable energy source because there is a huge demand for green energy. Solar energy is a promising future technology since it is clean and good for the environment [1, 2]. There are many different types of solar cells, including amorphous silicon, cadmium telluride, copper indium gallium selenide, dye-sensitized, hybrid, monocrystalline, nanocrystal, and perovskite solar cells [3]. Third-generation (emerging technology) perovskite solar cell is the one that was chosen. The light-harvesting active layer of a perovskite solar cell is made of a material with a perovskite structure; generally, this material is a hybrid organic-inorganic lead- or tin-based compound [4, 5]. CH3NH3PbI3 is the most popular perovskite absorber and has an optical band gap that varies from 1.6 eV to 2.3 eV [6–12]. Lead perovskite halide shows the highest solar energy conversion efficiency at 23%. It however suffers from toxicity issues. Lead-free perovskites have been shown as a viable candidate for potential use as light harvesters to ensure renewable PV technologies, where the lead can be replaced with Sn, Ge, Bi, Sb, and Cu. The candidates reported efficiencies of up to 9%; however, their efficiency and stability in the air are still urgently needed to be enhanced [13].

To date, researchers have made efforts in contributing to the development of perovskite semiconducting materials which have led to the rise of low cost and high efficiency concerning the simulation of the solar cell capacitance simulator-one dimension (SCAPS).
In this case study, we introduce a Sn-based perovskite structure that has high efficiency compared to previously submitted cells and is ecofriendly. Currently, tin-based PSCs demonstrate a maximum PCE over 13% together with excellent device stability, making them a very attractive photovoltaic technology to be further developed in the near future [14]. Since tin-based perovskite solar cells are affected by the oxidation process they tend not to be stable in the surrounding atmosphere. Hence, the measured efficiency of the perovskite solar cells decreases drastically with time. Researchers attempted to solve this issue by adding SnF2 to the perovskite structure. Several studies have been conducted in recent years, both simulation and experimental, with CH3NH3SnI3-based solar cells. A simulated research work published in 2021 achieved a JSC of 31.66 mA/cm², VOC of 0.96 V, FF of 67%, and a conversion efficiency of 20.28% [15]. Then, another work published in 2016 has a JSC of 31.59 mA/cm², VOC of 0.92 V, FF of 79.99%, and conversion efficiency of 23.36% [16]. In 2019, the work had a conversion efficiency of 23.76% [17]. For the proposed (Zn2SnO4/CH3NH3SnI3/Ni) structure, the obtained conversion efficiency in 2021 is 24.73% [18]. In 2017, it had a conversion efficiency of 24.82%, JSC of 25.67 mA/cm², FF of 78.14% and VOC of 1.0413 V [19]. The conversion efficiency of 26.33%, along with the VOC of 0.98 V, JSC of 31.93 mA/cm², and FF of 84.34%, have been reported for 2021 [20]. In 2021, another study obtained a conversion efficiency of 26.92% VOC of 0.99 V, JSC of 36.81 mA/cm², and FF of 73.80% [21]. In experimental works, two structures have been mentioned that obtained conversion efficiency of 17.1 and 15.1%. The structures are ITO/PEDOT: PSS/CH3NH3SnI3/C60/BCP/Ag and FTO/TiO2/Perovskite/Spiro-MeOTAD/Ag [22, 23]. After studying several valuable works, a novel structure (Al/ZnO/SnO2/CH3NH3SnI3/Ni) has been proposed in this research.

In this study, SnO2: F (fluorine-doped tin oxide) is used as a buffer layer because of the high transparency of the tin oxide semiconductor. F-doped SnO2 is the least expensive transparent conductive oxide material with the highest work function, the best contact with P-Si, thermal stability, chemical durability, a wide band gap, and negligible toxicity [24]. Due to its high conductivity, electron mobility, photocorrosion resistance, and low cost, zinc oxide (ZnO) has been recognized as a helpful electron transport material for solar cell applications [25].

The Sn-based perovskite solar cell is an HTL-free perovskite solar cell. HTL-free devices can greatly save the cost of materials. On the other hand, devices based on HTL-free configurations can reduce the fabrication cost, interface defects without affecting cell performance, and the complexity of processing because fewer layers are used [14].

2. Device Architecture and Numerical Simulation

The proposed Sn bead solar cell structure, which has the composition Al/ZnO/SnO2/CH3NH3SnI3/Ni, is shown schematically in Figure 1. Figure 1 shows that Ni was used as the back contact, CH3NH3SnI3 was used as the absorber layer, SnO2 was chosen as the buffer layer, and ZnO was used as the ETL for this perovskite solar cell.

Researchers from the University of Gent’s Electronics and Information Systems (ELIS) Department created the numerical simulation tool known as SCAPS [26]. SCAPS-1D uses two essential semiconductor equations: the continuity equation for electrons and holes under steady-state circumstances and the Poisson equations (27)–(34). Poisson’s and continuity equations are applied to free electrons and holes in the conduction and valence bands.

The following are the continuity equations for electrons and holes:

\[
\frac{dJ_n}{dx} = G - R, \quad (1)
\]

\[
\frac{dJ_p}{dx} = G - R, \quad (2)
\]

where \(J_n\) and \(J_p\) represent electron and hole current densities, \(R\) represents the recombination rate, and \(G\) represents the generation rate. The Poisson equation is as follows:

\[
\frac{d^2\Psi}{dx^2} = \frac{e}{\varepsilon_o \varepsilon_r} \left( \rho(x) - n(x) + N_D - N_A + \rho_p - \rho_n \right),
\]

where \(\Psi\) is the electrostatic potential, \(e\) is the electrical charge, \(\varepsilon_r\) is the relative permittivity, \(\varepsilon_o\) is the vacuum permittivity, \(\rho\) and \(n\) are the hole and electron concentrations, \(N_D\) is the donor type, \(N_A\) is the acceptor type charged impurities, and \(\rho_p\) and \(\rho_n\) are the hole and electron distributions, respectively [19, 35]. The physical parameters needed for the simulation are shown in Table 1.

3. Results and Discussions

3.1. J–V and Q–E Curve of Sn-Based Perovskite Solar Cell

Figure 2 shows the designed solar cell’s J–V characteristics and different absorber thicknesses. The absorber layer thickness varied from 0.1 μm to 3.0 μm, respectively. Current and voltage...
rise with increasing absorber thickness, as shown by the $J-V$ curve in Figure 2. Improved current and voltage result from adding the electron-hole pair while thickening the absorber.

Figure 3 shows the wavelength versus quantum efficiency. Quantum efficiency is defined as the ability of a solar cell to absorb carriers from incident photons of a specific energy. As can be seen, the thinner the absorber, the fewer photons at longer wavelengths are absorbed. This is because photons form fewer electron-hole pairs inside the absorber layer [20]. With a thick absorber layer, solar cells operate more efficiently because the likelihood of back recombination is reduced, which enhances the quantum efficiency [38]. Moreover, light is not absorbed below band gaps for longer low-energy wavelengths, resulting in a quantum efficiency of zero for wavelengths greater than 950 nm. The light-absorbing layer’s thickness considerably influences perovskite solar cell performance [16, 39–41].

To evaluate the effectiveness of the suggested CH$_3$NH$_3$SnI$_3$-based perovskite solar cell, the absorber’s thickness is changed from 0.5 to 3.0 μm. As the absorber layer thickness increased, all solar cell output metrics significantly increased, as shown in Figure 4. The value of $V_{OC}$ rose from 0.920 to 0.982 V, $J_{SC}$ from 32.150 to 35.123 mA/cm$^2$, FF 80.76 to 86.02%, and efficiency from 23.89 to 29.68% likewise increased while varying the absorber thickness from 0.5 to 3.0 μm.

It is proposed that the photogenerated electrons and holes will be significantly boosted at thicker absorber layers, improving the overall performance of the solar cell. As a result, considering the device manufacturing cost, the CH$_3$NH$_3$SnI$_3$ absorber thickness is set at 1.5 μm in this study, which is chosen as the best thickness for further research.

3.2. Impact of Acceptor Density and Defect Density of the Absorber Layer. Figure 5 displays the solar cell output parameters $V_{OC}$, $J_{SC}$, FF, and efficiency. In this study, we...
discovered that as acceptor density increased, so did the $V_{OC}$, FF, and efficiency. When the acceptor density is increased, the $J_{SC}$ decreases. The acceptor density has been changed from $10^{11}$ to $10^{17}$ cm$^{-3}$. The $V_{OC}$ varies from 0.913 to 1.081 V, $J_{SC}$ from 35.178 to 31.559 mA/cm$^2$, FF from 84.41 to 86.66%, and efficiency from 27.12 to 29.58%, while the acceptor densities have changed from $10^{11}$ to $10^{17}$ cm$^{-3}$, respectively. The absorber layer acceptor density influences the performance of photovoltaic systems. This computational study looks at how the proposed CH$_3$NH$_3$SnI$_3$-based perovskite solar cell reacts to absorber layer acceptor density changes.

The defect density in the absorber significantly impacts the performance of photovoltaic systems. Another critical factor that might affect the device’s performance is the active layer’s total defect density. Figure 6 illustrates the numerical study's investigation of the proposed Sn-based perovskite solar cell reaction to changing defect densities in the absorber layer related to the intended perovskite solar cell $V_{OC}$, $J_{SC}$, FF, and efficiency values. The absorber layer’s defect density varied from $10^{14}$ to $10^{18}$ cm$^{-3}$. The $V_{OC}$ decreased from 0.957 to 0.625 V, $J_{SC}$ from 34.604 to 10.863 mA/cm$^2$, FF from 83.88 to 39.96%, and efficiency from 27.79 to 2.71% when defect density varied from $10^{14}$ to $10^{18}$ cm$^{-3}$. More significant pinhole production and recombination due to increased film deterioration decreased stability and reduced device performance are all effects of higher defect concentrations in the absorber layer [42]. We conclude that an increase in defects results in a reduction in the charge carriers’ diffusion length and an increase in recombination carriers in the absorber layer, which directly impacts efficiency [43].

### 3.3. Impact of Series ($R_s$) and Shunt ($R_{sh}$) Resistances

The performance of Sn-based perovskite solar cell structures is significantly influenced by series ($R_s$) and shunt ($R_{sh}$) resistances. The resistance $R_s$ between various terminals on the front and back contacts of the cell is the sum of these resistances. The series resistance ($R_s$) is produced by the active junction’s reverse saturation current caused by manufacturing faults. Using the SCAPS-1D simulator, the impact of $R_s$ and $R_{sh}$ on solar cell performance, such as $V_{OC}$, $J_{SC}$, FF, and efficiency, has been assessed as a function of $R_s$, as shown in Figure 7. The performance is examined by changing $R_s$ between 0 and 5 $\Omega$-cm$^2$ while $R_{sh}$ is constant at $10^3$ $\Omega$-cm$^2$.

Figure 7 demonstrates that the efficiency and FF dramatically dropped when the $R_s$ increased. When $R_s$ was increased from 0 to 5 $\Omega$-cm$^2$, the efficiency decreased from 28.18 to 22.93% and the FF from 84.60 to 68.97%. The results achieved in this simulation are identical to prior research.
conclusions [44, 45]. At the same time, $J_{SC}$ and $V_{OC}$ are almost constant, as shown in Figure 7. $J_{SC}$ obtained 34.63 to 34.55 mA/cm$^2$, $V_{OC}$ increased 0.961 to 0.962 V while $R_S$ varied from 0 to 5 $\Omega$-cm$^2$. Figure 8 shows the output parameters as a function of $R_{sh}$ for the proposed perovskite solar cell. With $R_{sh}$ being changed from $10^6$ to $\Omega$-cm$^2$ and $R_S$ remaining constant at 0.5 $\Omega$-cm$^2$, the impact of $R_{sh}$ is examined. The $V_{OC}$ increases from 0.344 to 0.961 V, $J_{SC}$ 32.978 to 34.627 mA/cm$^2$, FF 25.01 to 83.02%, and efficiency 2.84 to 27.65% along with the increase of $R_{sh}$.

3.4. Impact of back Contact Work Function and Operating Temperature. To generate a moderate built-in potential there, a material with a suitable work function at the back contact properties of the recommended cell is investigated, as illustrated in Figure 9. The back contact work function varied from 4.4 to 5.4 eV. Figure 9 shows that $V_{OC}$, FF, $J_{SC}$, and efficiency rise as the work function is raised. The $V_{OC}$ is increased by 0.143 to 0.966 V, $J_{SC}$ 33.455 to 34.728 mA/cm$^2$, FF 54.55 to 84.89%, and efficiency 2.61 to 28.48%. The performance of solar cells is observed to be significantly impacted by the back contact work function. According to the current modelling findings, a work function more significant than 5.1 eV is required for adequate PV performance. Because of its reasonable cost and essential work function, nickel (Ni = 5.35 eV) has been utilized as the back contact in this numerical study to achieve the high performance of a CH$_3$NH$_3$SnI$_3$-based solar cell [46].

The device simulations were conducted at an operating temperature of 300 K. Under steady light of 1000 Wm$^{-2}$, the device’s operating temperature was changed from 295 to 425 K to examine the effects of temperature on perovskite solar cells. Figure 10 shows the device parameters as a function of temperature. Figure 10 shows that the output parameters of $V_{OC}$, FF, and efficiency are decreasing, and $J_{SC}$ is almost stable in this investigation. For perovskite solar cells, working temperature is an important consideration. Mainly, there is a high correlation between operating temperature and metrics like $J_{SC}$ and $V_{OC}$ [47]. The $V_{OC}$ is obtained at 0.968 to 0.770 V, $J_{SC}$
34.633 to 34.705 mA/cm², FF 84.71 to 79.19%, and efficiency 28.42 to 21.18%, while the temperature of the proposed structure has varied from 295 to 425 K. The $V_{OC}$ decreases due to a rise in device temperature, which also causes exponential growth in the reverse saturation current [48]. Because there are fewer free carriers in the cell due to the increase in the recombination rate of photogenerated carriers, such as electrons and holes, the performance of the cell as a whole decrease at higher temperatures [49].

Figure 7: Impact of series resistance on $V_{OC}$, $J_{SC}$, FF, and efficiency.
Figure 8: Impact of shunt resistance on $V_{OC}$, $J_{SC}$, FF, and efficiency.

where, $R_S = 0.5$ (Ω- cm²)

Figure 9: Impact of the back contact work function on $V_{OC}$, $J_{SC}$, FF, and efficiency.
4. Conclusions

In this study, Sn-based perovskite solar cell structure (Al/ZnO/SnO2/CH3NH3SnI3/Ni) has been investigated and simulated using SCAPS-1D software. The absorber layer thickness varied from 0.5 to 3.0 μm, acceptor density $10^{11}$ to $10^{17}$ cm$^{-3}$, defect density $10^{14}$ to $10^{16}$ cm$^{-3}$, series ($R_s$) 0 to 5 Ω-cm$^2$ and shunt ($R_{sh}$) $10^1$ to $10^6$ Ω-cm$^2$, back contact work function 4.4 to 5.4 eV, and the operating temperature 295 to 425 K as shown on the output parameters of the solar cell. The optimum thickness of the absorber layer is 1.5 μm and 0.05 μm for the buffer layer. The proposed Sn-based perovskite solar cell structure has obtained a conversion efficiency of 28.19% along with FF of 84.63%, $J_{SC}$ of 34.634 mA/cm$^2$, and $V_{OC}$ of 0.961 V. Moreover, the conversion efficiency decreases with an increase in operating temperature. Due to the absence of harmful components, this structure is also excellent for the environment. So, we hope it will be an efficient and ecofriendly perovskite solar cell for fulfilling the upcoming generation’s demands.

Data Availability

The data supporting the investigation’s results are available upon reasonable request from the relevant author.

Conflicts of Interest

The authors state that they have no conflicts of interest.

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References


