Impact of HTM on Lead-free Perovskite Solar Cell with High Efficiency

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Abstract

The Scaps-1d simulator was used to simulate a lead-free perovskite $\text{CH}_3\text{NH}_3\text{SnI}_3$ based solar cell devices fabricated from different hole transport materials (HTM). This research looks at two organic and two inorganic HTM layers. The cell structure used in this study is $\text{FTO}/\text{TiO}_2/\text{CH}_3\text{NH}_3\text{SnI}_3/\text{HTM}(\text{variable})/\text{Au}(\text{variable})$. Spiro-OMeTAD, PEDOT:PSS, CuO and Cu_2O are the HTM materials used. The results show that utilizing CuO as an HTM produces better outcomes than other HTMs, with an efficiency of 28.45%. The thickness, acceptor concentration (N_A), and defect density (N_t) of the perovskite layer on optoelectronic properties of the solar cell are focus of simulation studies. According to this study, an perovskite layer thickness of 1000 nm is suitable for a decent photovoltaic cell. Furthermore, by adjusting the HTM thickness and the defect density of HTM and absorber layer, promising findings of J_{sc} of 34.38 mAcm^{-2} , V_{oc} of 1.011 V, FF of 80.85% and PCE of 28.10% were obtained for Spiro-OMeTAD based PSC. Finally, in order to improve the device's performance, an anode material with high work function is required. Our findings reveal that using a thin absorber layer results in low photo generated charge carriers due to less absorption, but high carrier extraction. Although more carriers are created in the cell due to increased absorption, decreased collection efficiency is related to recombination, which decreases V_{oc} for thick perovskite layers. Device efficiency is improved by increasing the doping density up to 10^{18} cm^{-3} in the perovskite layer due to built-in electric field across the solar cell. Again a very thin or thick HTL is not ideal for high PCE. For low recombination and a high fill factor, an HTM (Spiro-OMeTAD) of 1–100 nm is necessary. The great power conversion efficiency of organic HTM based lead-free PSC brings up the new possibilities for obtaining renewable energy.

1. Introduction

The need for energy will skyrocket in the future. The majority of today's energy usage is derived from fossil fuels, which will be depleted in the near future and it pollutes our environment. Because of this the renewable energy sources are in high demand as a result of industrialization and population growth. Solar energy is a promising source for this because it has no negative impact on our environment [1–7]. Photovoltaic devices are required as a part of a long-term global energy strategy. The energy research community has been paying close attention to perovskite solar cells as their has improved PCE day by day. Efficiency of this cell was relatively low at the initial time. But recently PSC's state of art certified PCE has a success rate of more than 25% [7–10]. Again, these perovskite materials have unique properties such as a high absorption coefficient, good charge carrier mobility, low exciton binding energy, and long charge carrier diffusion length [9, 11–13]. As a result, it is indispensable to work on it. The photovoltaic effect can be used to transform this energy into electricity [14]. It is, however, a cheap and clean source of energy, and as a result, it has dominated the photovoltaic market for Si-based solar cells [15]. Because of their excellent solar cell PCE, researchers investigated pure and modified methyl ammonium lead halide as a perovskite material[16, 17]. Lead-based electronic equipment, on the other hand, have been strictly regulated by the European Union and other countries. The power conversion efficiency of these materials

was extremely high. Lead, on the other hand, is not environmentally friendly and is damaging to both individuals and environment [18–25].

To address this issue, several scientists and researchers have looked into the lead-free perovskite $\text{CH}_3\text{NH}_3\text{SnI}_3$ as a photovoltaic material due to the excellent optoelectronic capabilities. This material has a straight band gap of 1.3 eV, lying in the range of the absorber. Several group of researchers have succeeded in fabricating organic-inorganic perovskite solar cells based on $\text{CH}_3\text{NH}_3\text{SnI}_3$. In this work we develop organic-organic eco friendly perovskite solar cells using two organic HTMs (Spiro-OMeTAD, PEDOT:PSS). The electron transport material (ETM) is an important part of the PSC. The proper energy level for electron injection, strong electron mobility, chemical stability, low synthesis cost, and environmental friendliness make TiO_2 an attractive candidate material [26–29]. The band gap of TiO_2 material is appropriate for reducing the transmission of holes [30]. In PSC, the hole transport material is crucial for achieving high PCE. For minimum recombination of charge carriers at the interface, HTM requires higher value hole carrier mobility with fewer defects at the HTM/absorber layer. Cu_2O as an HTM has recently been reported by Yu et al. to have strong hole mobility and appropriate energy level configuration with $\text{CH}_3\text{NH}_3\text{SnI}_3$ and photo-generated charges with higher life time [28]. It lowers the metal contact barrier height and lowers minority recombination loss at the anode. Because of this Cu_2O is employed as an HTM. P Swaicka-Chudy et al reported that as a HTM layer CuO provided better efficiency in solar cell than Cu_2O [31]. Because of this we have chosen CuO as a HTM.

In this solar cell structure absorber layer is sandwiched between ETM and HTM where FTO and Au used as front and back electrode. A TiO_2 layer is utilized as an ETL towards the front electrode. Organic HTM is a Spiro-OMeTAD layer above the absorber that blocks electrons while allowing holes to flow towards the back electrode. Among all the organic HTM materials Spiro-OMeTAD is the most frequently used and benchmark material for high PCE solar cells. This is owing to $\text{CH}_3\text{NH}_3\text{SnI}_3$ perfect energy band alignment and great transparency of visible light [32]. HTM not only aids hole conveyance, but it also prevents the contact between the back electrode and the absorber. The likely hood of collecting holes is determined by the thickness of HTM. As a result for high PCE solar cell HTM thickness optimization is required.

The conductivity of spiro-OMeTAD is about 3.5×10^{-7} S/cm [33] which is quite low. However, the conductivity of p-type spiro-ometad is higher than that of intrinsic Spiro-ometad. When spiro-OMeTAD is utilised, high J_{sc} and V_{oc} are obtained, indicating that Spiro-OMeTAD has a high charge collection efficiency. The quasi-Fermi level difference between ETM (TiO_2) and HOMO level of HTM (Spiro-OMeTAD) is responsible for the higher value of V_{oc} [34]. V_{oc} can be increased by lowering the HOMO energy level. Using Spiro-OMeTAD we have achieved a high FF with low series resistance (R_s) and high shunt resistance (R_{sh}).

Fill factor (FF), R_s , and PCE are all determined by the thickness of the absorber, ETL, and HTL. Around 120 nm of compact TiO_2 is adequate for ETL. As a result of our prior findings, we may conclude that when thickness of the TiO_2 layer grows, then cell's R_s grows. As a result, light transmission through TiO_2

diminishes. The latter diminishes J_{sc} and PCE by affecting photogeneration in the perovskite layer. Fill factor falls as series resistance rises, and PCE suffers as a result. In addition, our research indicated that a doping density of $10^{18} / \text{cm}^3$ was appropriate for high fill factor TiO_2 . Various thicknesses are reported for perovskite (absorber) and HTM layers, and an optimal value for each layer is necessary. A thick (> 1000 nm) perovskite layer results in reduced hole collection efficiency due to an increase in R_s and recombination inside the perovskite layer. A very thin (< 100 nm) perovskite layer causes low photocurrent because of less photo absorption. The probability of recombination is reduced since holes travel a shorter distance to reach the back electrode, device performance is improved when a thinner HTM (0.1–10 nm for Spiro-OMeTAD) is utilised. Despite this, an extremely thin HTM reduces the device's repeatability and stability because the counter electrode can penetrate through the HTM and touch the perovskite layer, shunting the device. But if we use a HTM of higher thickness which uniformly cover the rough perovskite layer, but it increases R_s and lowers μ_h . Furthermore, because $\text{CH}_3\text{NH}_3\text{SnI}_3$ contains crystallites, perovskite crystals can protrude through the HTM and contact the back electrode if a very thin HTL is utilised. To achieve a flat surface, HTL must be of an appropriate thickness which can cover the crystallites without altering the cell's R_s [35]. Moreover, a good HTM thickness improves the chances of collecting holes. If the layers are deposited using a spin-coating approach, the thickness of the layers can be adjusted by changing the spin-coating speed. To tune fill factor, energy band alignment, carrier concentration, and PCE, suitable doping in the $\text{CH}_3\text{NH}_3\text{SnI}_3$ absorber and Spiro-OMeTAD is necessary. In the absorber layer, dopants such as Mg, Na, Sn etc were utilised [36–38]. The Mg dopant in $\text{CH}_3\text{NH}_3\text{SnI}_3$ lowered the conduction band and valance band levels to those of TiO_2 conduction band and Spiro-OMeTAD valance band, respectively. Magnesium doping enhanced the grain size, resulting in a pinhole-free film [35]. The grain size of $\text{CH}_3\text{NH}_3\text{SnI}_3$ was similarly enhanced by sodium doping, and pin-hole-free films were formed. Doping with tin is less difficult than doping with bismuth or titanium. The $\text{CH}_3\text{NH}_3\text{SnI}_3$ band gap can be changed by changing the Sn doping concentration [35].

Spiro-OMeTAD is commonly utilised for hole transfer. The impact of Spiro-OMeTAD and $\text{CH}_3\text{NH}_3\text{SnI}_3$ layer thickness and doping density on solar cell characteristics is investigated in this paper. With the cell design of FTO/ETM/perovskite absorber/HTM/Au, its impact on solar cell characteristics is examined. High PCE solar cells are created via device modelling, which involves selecting an appropriate HTM and fine-tuning variables such as HTM thickness and doping density, as well as the active layer thickness and doping density. For this purpose we have used four different HTMs (Spiro-OMeTAD, PEDOT:PSS, CuO and Cu_2O). In results and discussion section, we present our findings.

2. Device Structure And Simulation Details

SCAPS 1d software was used to perform a simulation of a Sn-based lead-free perovskite solar cell in this study. This simulation was carried out with a 1000 W/m^2 light source. We have investigated this study at 300 K and an air mass of AM 1.5G. In the configuration of the reported solar cell HTM is p-type CuO

(variable), the absorber layer is $\text{CH}_3\text{NH}_3\text{SnI}_3$, and the n-type TiO_2 as an ETM, it's used. In addition, FTO was chosen as the contact material, while anodes made of Ag, Cu, Au, and Pt were chosen.

Tables 1 and 2 summarise material parameters derived from previous literature [39–41]. As shown in Table 1, the thickness of FTO (500 nm), TiO_2 (120 nm), and CuO (100 nm variable) were initially tuned for high PCE. Experimental results [15, 31, 42–45] were used to calculate the absorption coefficients of FTO, CuO, Cu_2O , Spiro-OMeTAD, PEDOT:PSS, $\text{CH}_3\text{NH}_3\text{SnI}_3$, and TiO_2 .

3. Results And Discussion

The energy band alignment and J-V graph of the reported PSC were displayed in Figs. 1a–b, respectively. For this, the used parameters shown in Tables 1 and 2. Inside the absorber layer, electron–hole pairs are formed after illumination. Electrons and holes travel towards ETL and HTL, respectively, due to the junction field. The cathode and anode collect the electrons and holes, respectively, and form a voltage. Using the initial electrical parameters the obtained values of J_{sc} V_{oc} , FF and PCE are 27.23 mA/cm^2 , 0.854 V, 71.08% and 16.54% respectively. We have determined the device's J_{sc} by the active material's absorption coefficient, thickness, and mobility. The photo current will be higher if the absorption coefficient is higher [9, 12, 41, 39, 46]. The thickness of the absorber is the second crucial factor. It must be thick enough to absorb the incident solar radiation's greatest cut off wavelength[40, 41]. Apart from that, movement is quite important for achieving a high J_{sc} . After illumination, the J_{sc} should be equivalent to solar cell current. For $\text{CH}_3\text{NH}_3\text{SnI}_3$ samples synthesised by open tube technique, Ma et al. and Stoumpos et al. showed extremely high value of μ_e (2000 cm^2/Vs) and μ_h (300 cm^2/Vs) [47, 48]. Lazemi et al. used similar values of carrier mobilities and reported a high value of J_{sc} (37 mA/cm^2) [42]. The mobility of electrons and holes in this simulation was based on research published recently [40, 47, 46, 48]. The high value of J_{sc} was reached because current density is linearly related to charge carrier mobility. Devi et al.[49] and Khattak et al.[50], on the other hand, used substantially lesser and identical values of μ_e (1.6 cm^2/Vs) and μ_h (0.16 cm^2/Vs) and reported good J_{sc} (30 mA/cm^2) results. Again we found in some previous experimental literature that diffusion length is directly proportional to the mobility's square root [51]. As a result, for high charge carrier mobility, diffusion length increases, and recombination of charge carriers reduces. There could be different causes for the greater J_{sc} when compared to recently published data [49, 50]. The performance of the reported PSC is promising and reliable with the Sn-based PSC [27, 29]. It is feasible to improve photovoltaic performance even more. PSC's energy band diagram is shown on Fig. 1a. At the absorber/ETL contact, we have observed a positive value of CBO which is roughly 0.35 eV. This positive spike blocks the flow of Photo-generated electrons towards the electrode [51–53].

3.1 Absorber thickness

The thickness of the absorber, as indicated in Fig. 2, is a limiting parameter for cell performance. The absorber layer thickness can be adjusted to improve cell efficiency. Photon absorption and carrier

collection have a reciprocal relationship in planar solar cells. The thickness of the absorber in this reported PSC ranged from 100 nm to 4000 nm. Photo generated current is minimal for 100 nm thin absorber layer. Charge extraction, on the other hand, is high, as demonstrated by the high V_{oc} , which indicates less recombination.

Figure 2(a), shows the increment of J_{sc} with absorber thickness due to better light absorption. It immediately climbs from 26.2 mA/cm² to 34.56 mA/cm² for an increment of thickness from 100 nm to 1000 nm, then decreases until all light is absorbed, at which point it saturates at 35 mA/cm². J_{sc} is quite low around 100–200 nm due to decreased absorption, and utilising thicker (> 1000 nm) sheets has no benefit. The maximum value of J_{sc} (~ 35 mA/cm²) observed for a thickness of 1000 nm is mostly owing to the perovskite's high value of absorption coefficient [41]. As a result, a 800–1000 nm absorber thickness is appropriate. Since R_s of the PSC increases, the fill factor falls with thickness. But a thick absorber surpasses the diffusion length and charge carriers are recombine.

Our findings demonstrate that the increase in J_{sc} of the PSC is just 6.25% when comparing thicknesses of 400 nm and 1000 nm. This signifies that, while more charge carriers are generated as a result of increased absorption, a thicker cell's collection efficiency is reduced because of high recombination, as a result there is a decrease in V_{oc} . This decrease in V_{oc} with shown in Fig. 2(b) is linked to a decrease in the effective band gap and an increase in recombination [40]. A decrease in V_{oc} as thickness grows could be owing to increased recombination. Increasing absorber thickness, a modest decrease in FF (Fig. 2c) indicates a raise in R_s in the PSC [41]. Cell efficiency (Fig. 2d) grows gradually until it reaches 1000 nm absorber thickness due to J_{sc} alone, while efficiency saturation is due to both absorption and J_{sc} . Due to small absorption of light and reduced photogeneration, efficiency around 100 nm is low. Because of the highest absorption of light beyond 1000 nm, PCE remains steady at 28.45%, as indicated by constant J_{sc} . From a non-optimized efficiency of 22.47 percent, an optimised thickness of 1000 nm increased efficiency to 28.45 percent. Adjusting the absorber thickness to 700–1000 nm results in excellent efficiency, according to our simulation.

3.2 Acceptor carrier concentration (N_A) of $CH_3NH_3SnI_3$

Apart from the $CH_3NH_3SnI_3$ layer thickness, the acceptor density of holes in the perovskite layer has a considerable impact on the device performance of photovoltaic cells. Sn^{2+} is transformed to Sn^{4+} when the device is exposed to air in $CH_3NH_3SnI_3$ oxides. But, this procedure degrades the device's PCE and converts it to a p-type semiconductor[47]. The formation of Sn^{2+} to Sn^{4+} is inhibited by the addition of SnO_2 [15, 46, 54]. Feng et al. used Hall-effect measurement to calculate the dark carrier density of 10^{14} cm⁻³ to 10^{17} cm⁻³ [55]. The hole concentration in this perovskite layer can be adjusted up to 10^{19} cm⁻³, according to Takashi et al [56]. As a result, the acceptor density of our reported perovskite layer was changed from 10^{14} cm⁻³ to 10^{19} cm⁻³ to see how acceptor doping concentration influences photovoltaic characteristics.

Cell characteristics for varied acceptor density in the $\text{CH}_3\text{NH}_3\text{SnI}_3$ layer are shown in Fig. 3 (a) and (b). For a very high acceptor density ($> 10^{19}/\text{cm}^3$), Auger recombination can be highly relevant. The device's V_{bi} can increase as the doping level rises above $10^{14}/\text{cm}^3$. Strong V_{bi} enhances photogenerated carrier separation and cell efficiency. Nonetheless, a high level of doping promotes Auger recombination and lowers V_{oc} . As a result, the maximum acceptor density in the perovskite layer in our study was set to $10^{18}/\text{cm}^3$. In addition, due to a high recombination rate, very high p-type doping levels in the perovskite layer can restrict hole transportation from the absorber to the HTL. In our situation, the doping density isn't particularly great, hence no change in J_{sc} or V_{oc} was detected. Simultaneously, increasing the acceptor density from 10^{14} cm^{-3} to 10^{19} cm^{-3} can develop the better device's V_{bi} . This high V_{bi} forces the charge carriers towards the electrodes and boosts the charge collection efficiency and FF. As a result, cell performance improves with doping density. Our findings demonstrate that for $N_A = 10^{14} / \text{cm}^3$ to $10^{18} / \text{cm}^3$ there is a continuous increase in FF and PCE, and then for $N_A = 10^{19} / \text{cm}^3$ FF and PCE decline rapidly from 81.26 to 62.17 and 28.30 to 22.81, respectively. So the optimized value of N_A of absorber layer is $10^{18}/\text{cm}^3$.

3.3 Defect density (N_t) at absorber

We also examined the influence of absorber defect density was. In the absorber layer, defects are unavoidable. They can be found both in the bulk and on the surface. Defects in the perovskite absorber layer that appear as point defects include lattice vacancies, interstitial, Schottky, and Frenkel defects. The impurity defect in the absorber layer is caused by the self-doping process [15, 47, 46, 55]. Deep or shallow levels in the energy band gap are introduced by these defects[57]. Charge carriers can trap and enhance nonradiative electron–hole recombination as a result of these imperfections [39, 40]. The diffusion length of charge carriers in Sn-based perovskite absorber layers can be extended up to $\sim 3 \mu\text{m}$ by employing a tin-reduced precursor solution[58]. Because charge carrier diffusion length is proportional to defect density[49]. To investigate the influence of electron diffusion length on photovoltaic responses, the defect density was changed from 10^{18} to 10^{14} cm^{-3} [59] and the electron diffusion length was adjusted from 0.046 to 4.6 μm . Lazemi et al and some other researchers [40, 39, 60] have all used a similar change in defect density. The defect density was altered from 10^{14} to 10^{16} cm^{-3} based on these research, and its influence on photovoltaic characteristics of the reported perovskite solar cell was displayed in Fig. 4.

It was discovered that as the defect density was reduced, the device's performance improved. The initial N_t of the perovskite layer was adjusted at $1 \times 10^{16} \text{ cm}^{-3}$. Because the diffusion length of electrons and holes for this N_t value is almost identical to empirically reported values [28]. The cell performance is greatly enhanced when the defect density is 10^{14} per cm^{-3} , with the values of J_{sc} , V_{oc} , FF and PCE are $34.17 \text{ mA}/\text{cm}^2$, 0.999 V, 80.68% and 27.54% respectively. Now, N_t has decreased even further, from 10^{14} to $0.5 \times 10^{14} \text{ cm}^{-3}$, with little variations in J_{sc} and FF, but significant changes in V_{oc} and PCE.

3.4 Metal work function

A work function research was conducted using various anode materials to investigate the ohmic or rectifying behaviour at the metal/HTM junction. For PSC simulations, different metals such as Ag (4.74 eV), Cu (5.0 eV), Au (5.1 eV), and Pt (5.7 eV) were used as anodes [61, 62]. Figure 5a,b shows the energy band alignment for different work function's metals as anode. As can be seen, the hole barrier layer grows as the work function of the contact materials decreases. The influence of the anode material on FF and PCE of the reported Perovskite solar cell PSC is shown in Figs. 5c,d. We can see that as the work function of the anode is reduced, PCE decreases. When the work function of the anode is less than CuO's work function, a rectifying Schottky barrier contact forms at the anode/CuO interface. As seen in Fig. 5a, this barrier obstructs the conduction of hole towards anode and lowering the fill factor with PCE. When the anode's work function is greater than the CuO's work function, an ohmic contact is produced at the anode/CuO junction. The hole transport at that interface is enabled by this ohmic contact. As a result, Jsc and PCE are showing signs of improvement.

3.5 Effect of HTM thickness

We have employed four distinct HTMs (CuO, Cu₂O, spiro-OMeTAD and PEDOT:PSS) and their thickness varying from 1 to 800 nm to investigate the effect of HTM thickness on optoelectronic capabilities. Except for spiro-OMeTAD, we found that HTM thickness has no effect on optoelectronic properties of the PSC. Figure 7 depicts the role of HTM (spiro-OMeTAD) thickness. HTM thickness affects cell performance in the same way that absorber thickness does. For high efficiency, a thickness of around 1–100 nm is optimal. With a thickness of 10 nm, the highest value of Voc, Jsc, FF, and PCE were 1.011 V, 34.38 mAcm⁻², 80.85%, and 28.10%, respectively. This suggests that the device has good charge transfer, less recombination, a high FF, and low R_s. HTM may not completely cover up the projecting perovskite crystals which are present in the perovskite layer if the thickness is less than the optimum thickness. Our simulated results reveal that no HTM, as well as less than 10 nm or more than 100 nm, is ideal for high PCE. V_{oc} reaches saturation and is independent of thickness when the HTM thickness is less than 10 nm. The device's V_{oc} and recombination are linked. V_{oc} can be influenced by factors that influence recombination, and this is true whether the HTM is thin (less than 10 nm) or not. A change in series resistance is indicated by a change in fill factor with HTM (spiro-OMeTAD) thickness. When the HTM thickness is increased from 0.1 nm to 10 nm, the fill factor rises to 80.85% and cell efficiency rises to 28.10%. When the thickness is increased to 800 nm, the FF and PCE are reduced to 73.19% and 25.46%, respectively. Because the path length of photo generated carriers to reach the bottom electrode is increased, raising R_s. A thin HTM (< 10 nm) does not completely cover the perovskite layer, increasing the likelihood of recombination. When the HTM thickness increases from 0.1 to 10 nm, the fill factor improves due to increased coverage. As a result of the rise in R_s with the thickness of HTL, the FF decreases.

3.6 Effect of secondary doping

By adding fresh dopants to the HTM, we may change the hole concentration, which has a secondary doping role in modifying the conductive polymer conduction. As a result, we investigated the effects of

hole concentrations in the range of 10^{14} – 10^{19} cm^{-3} on the photovoltaic parameters of the PSC, and the findings are shown in Fig. 7. In general, polymer doping is done to enhance charge carrier density and μ_h . However, a large quantity of doping reduces μ_h . As a result, the secondary doping density must be tuned such that the cell's performance is not harmed. We can only raise the efficiency of the Spiro-OMETAD HTM based PSC by increasing the hole density. Acceptor concentration was tuned from 10^{14} to 10^{19} cm^{-3} to explore the effect of HTL doping density, and the results are presented in Fig. 7. Because of improvements in conductivity of HTL, the fill factor improves to 80.85. Fill factor reaches to this maximum value when the doping density is 1×10^{18} cm^{-3} . When the acceptor doping level was equivalent to 10^{18} cm^{-3} , we were able to attain a high PCE of 28.10% with V_{oc} , J_{sc} , and FF of 1.011 V, 34.38 mA cm^{-2} , and 80.85%. Finally, Fig. 8 shows the optimized J vs V characteristics of a spiro-OMeTAD HTM based PSC.

3.7 Effect of temperature

Another key aspect that affects the performance of PSC is temperature. The temperature of the PSC rises with absorption of light, thus temperatures are frequently greater than 300 K. In this work, we varied a temperature from 300 to 360 K and plotted the photovoltaic parameters against it (Fig. 9). Where increasing the temperature lowers the V_{oc} and PCE. But increasing temperature increases FF and J_{sc} . The efficiency of all samples decreased as the temperature increased, which could be explained by the fact that at higher temperature, the electron absorbs more energy and goes to an unstable state, which increases the rate of recombination and lowering the PCE of the PSC [63, 64].

3.8 Comparative study

We picked two organic and two inorganic HTMs to construct four distinct PSCs for a comparative investigation. The PSC structure is unchanged in this investigation; only the HTM layer is altered. We picked a thickness of 300 nm for all HTM layers in this work. Table 3 summarizes the simulation findings, which indicate the impact of HTM layers on PSC performance. This demonstrates that CuO outperforms all other HTM in terms of efficiency. The spiro-OMeTAD HTM based PSC has a 28.10% efficiency in the optimal condition, with V_{oc} , J_{sc} , and FF values of 1.011, 34.38, and 80.85, respectively.

Table 1
The optoelectronic simulation parameters.

Parameters	FTO	TiO ₂ (ETM)	CH ₃ NH ₃ SnI ₃ (absorber)	Cu ₂ O	CuO	Spiro-OMeTAD	PEDOT:PSS
Thickness(nm)	500	120	800 (variable)	300	800	10 (variable)	300
E _g (eV)	3.4	3.2	1.3	2.17	1.51	3.06	2.2
X (eV)	4.5	4.1	4.17	3.2	4.07	2.05	3.6
ε _r	9.1	9.0	8.2	7.1	18.1	3	10
N _c (cm ⁻³)	1.1 x 10 ¹⁹	2.2 x 10 ¹⁸	1 x 10 ¹⁸	2x10 ¹⁷	2.2 x 10 ¹⁹	2.8x10 ¹⁹	10 ¹⁹
N _v (cm ⁻³)	1.1 x 10 ¹⁹	1.8 x 10 ¹⁹	1 x 10 ¹⁸	1.1x10 ¹⁹	5.5 x 10 ²⁰	10 ¹⁹	10 ¹⁹
μ _n (cm ² /Vs)	20	0.05	2000	200	100	10 ⁻⁴	100
μ _p (cm ² /Vs)	10	0.05	300	80	0.1	2x10 ⁻⁴	0.4
N _D (cm ⁻³)	1.1 x 10 ¹⁹	1 x 10 ¹⁸	0	0	0	0	0
N _A (cm ⁻³)	0	0	1 x 10 ¹⁴ (variable)	1 x 10 ¹⁸	10 ¹⁸	10 ¹⁸	10 ¹⁸
V _e (cms ⁻¹)	10 ⁷	10 ⁷	10 ⁷	10 ⁷	10 ⁷	10 ⁷	10 ⁷
V _h (cms ⁻¹)	10 ⁷	10 ⁷	10 ⁷	10 ⁷	10 ⁷	10 ⁷	10 ⁷

Table 2
Parameters for the defects

Parameters	TiO ₂ (ETM)	CH ₃ NH ₃ SnI ₃	CuO
Defect type	Neutral	Neutral	Neutral
σ_n	1×10^{-15}	2.5×10^{-15}	1×10^{-15}
σ_p	1×10^{-15}	8.5×10^{-15}	1×10^{-15}
Energy distribution	Single	Gaussian	Single
Energy level with respect to E_v (above E_v) (eV)	0.6	0.65	0.1
Characteristic energy	-	0.1	-
N_t (cm ⁻³)	1×10^{14}	1×10^{16} (variable)	1×10^{14}

Table 3
The performance of PSCs made with various HTMs is summarized.

HTM	Thickness(nm)	V_{oc} (V)	J_{sc} (mA/cm ²)	FF (%)	PCE (%)
CuO	300	1.013	34.56	81.27	28.45
Cu ₂ O	300	1.011	34.51	81.19	28.34
PEDOT:PSS	300	1.0134	34.52	81.25	28.43
Spiro-OMeTAD	300	1.011	34.38	78.01	27.12
Spiro-OMeTAD	10	1.011	34.38	80.85	28.10

4. Conclusion

The Scaps-1d simulator was used to simulate a planar type lead free perovskite solar cell in this study. Several criteria, including perovskite layer thickness, N_A of absorber, N_t at absorber, and work function of anode, were used to optimize photovoltaic characteristics. The absorber and HTM thicknesses and doping densities were changed to see how they affected V_{oc} , J_{sc} , fill factor, and efficiency. Cell efficiency rose from 22.47–28.45% depending on perovskite layer thickness between 100 and 1000 nm, owing primarily to an increase in J_{sc} from 26.26 mAcm⁻² to 34.56 mAcm⁻². J_{sc} and PCE increase more slowly beyond 700 nm and saturate at 1000 nm due to saturated light absorption. Because photo generated charge carriers generated at the layer's centre will recombine when the thickness surpasses the diffusion length, long wavelength photon absorption due to band gap decrease in thicker films will be useless. The

rise in J_{sc} between 400 and 850 nm is only 6.2%, yet the increase in absorption is 18%. This demonstrates that not all produced carriers reach their intended electrodes. According to our findings, a perovskite layer thickness of 800 to 1000 nm is adequate for device application, and there is no benefit to using a thicker layer. Cell characteristics are also influenced by HTL thickness and secondary doping.

We investigated the performance of lead-free PSCs made from two organic and two inorganic HTMs in this work. Our findings demonstrate that among polymer HTMs, PEDOT:PSS with PCE of 28.43% outperforms Spiro-OMeTAD with a 28.10% efficiency. Furthermore, CuO, with a photovoltaic efficiency of 28.45%, outperforms Cu_2O , which has a PCE of 28.34% among inorganic HTMs. The capacity to apply secondary doping and build flexible solar cells is a significant benefit of organic HTMs. In terms of secondary doping in conductive polymers, we can conclude that secondary doping in Spiro-OMeTAD can effectively boost efficiency.

Declarations

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Author contributions

AKD was in charge of all experimental activities, data collection and analysis, and the first draught of the manuscript. The final version of the manuscript was approved. The manuscript was revised by Dr. RM. Dr. DKM revised the manuscript and gave his approval to the final version.

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Data availability

On reasonable request, the corresponding author will provide the datasets generated during the current work.

Conflict of interest

There are no conflicts of interest declared by the authors.

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Figures

Figure 1

(a) Energy band diagram and (b) J_{sc} vs V

Figure 2

Impact of absorber thickness (a) on J_{sc} , (b) on V_{oc} , (c) on FF and (d) on PCE

Figure 3

Influence of absorber doping density on (a) PCE and (b) J_{sc} .

Figure 4

Influence of defect density on (a) J_{sc} , (b) V_{oc} , (c) FF and (d) PCE

Figure 5

(a) Energy band alignment of the PSC for low work function Ag as anode, (b) EB of the PSC for high work function Pt as anode, (c) FF vs anode work function and (d) PCE vs work function.

Figure 6

Contour plot of PCE for CuO as HTM.

Figure 7

Represents the variation of PCE with thickness and N_A of spiro-OMeTAD

Figure 8

Jvs V characteristics of led free Perovskite solar cell using spiro-OMeTAD as HTM.

Figure 9

Impact of temperature on (a) J_{sc} , (b) V_{oc} , (c) FF and (d) PCE for CuO based PSC.