Optimization of highly efficient and eco-friendly EA-substituted tin based perovskite solar cell with different hole transport material

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Abstract
In this study, an EA-substituted tin based perovskite solar cell with different hole transport material (PEDOT: PSS, Cu2O, CuI, CZTSe) have been investigated using device simulation software. The effects of absorber thickness, defect density, operating temperature, J–V characteristics, and Quantum efficiency have been considered to enhance the performance of the solar cell. To confirm the feasibility and validate the study, all the simulation results were compared with reported experiment data. According to the experimental work based on (FA0.9EA0.1)0.98EDA0.01SnI3 absorber layer, a maximum of 13% efficiency is achieved with PEDOT: PSS as the HTM. Whereas we have further optimized performance parameters and found the superior response (Voc = 0.8851 V, Jsc = 27.24 mA/cm², FF = 77.91%, and PCE = 18.78%) while opted Cu2O as the hole transport material. This device structure FTO/Cu2O/(FA0.9EA0.1)0.98EDA0.01SnI3/IDL/PCBM/C60/Au provides the more efficient, reliable solution for replacing the lead-based perovskite solar cell. This study will aid researcher in a reasonable choice of materials and to predict the behavior of high performance solar cells before undergoing the fabrication process.

Keywords Lead-free perovskite solar cell · Absorber layer · Hole transport layer · Recombination · Defect density · Simulation

1 Introduction
The demand for clean and renewable energy is increasing each day. With the increasing demand for energy consumption, solar power is considered one of the promising technologies. Solar cell is a device that is used to convert solar energy into electricity (Sahli et al. 2018; Jiang et al. 2019). The monocrystalline and polycrystalline are the first-generation solar cells that are currently engaged in industrial applications due to its high efficiency.
But due to its high cost, large operation voltage, and environmental pollution leads to second generation solar cells (Bouich et al. 2021a; "High efficiency mesoscopic solar cells using CsPbI3 perovskite quantum dots enabled by chemical interface engineering." 2020). Cadmium telluride and copper indium gallium selenium thin-fil solar cells achieved good efficiency but again the production cost is high. Perovskite Solar cells (PSCs) have shown excellent performance nowadays. It has been grabbing the attention of researchers worldwide due to its high-power conversion efficiency. As of now, lead-based PSCs have achieved power conversion efficiency of 26.1% (Yang et al. 2017; Haase et al. 2018). Perovskite solar cells after attaining high conversion efficiency come up as a strong competitor of silicon-based solar cells in the photovoltaic industry (Zhou et al. 2018). Therefore, several considerable efforts have been done to replace toxic elements with non-toxic elements like Bi, Ge, Ag, and Sn (Punetha and Pandey 2020). Among all these alternatives, Sn is considered the best substitute of lead in perovskite solar cells due to its excellent optoelectronic properties and low band gap (Hasan et al. 2020). Sn overcomes the toxicity problem, is considered an eco-friendly solar cell, and provides good efficiency (Punetha et al. 2020). Research is still going on to overcome the instability issues of tin-based solar cells. Researchers are adding various components in the absorber layer to overcome the instability issues (self-doping) of tin-based perovskite solar cells. EA-substituted tin-based solar cell is one of the most stable and environment-friendly devices.

Implementation of various tin-based absorber layers like CsSnI3, FASnI3, and MASnI3 has come up with a solution of replacing toxic element lead (Pb) (Jing, et al. 2020). These layers provide an optimized power conversion efficiency of 9.10%, 9.99%, and 12.90% respectively (Dixit et al. 2021). Manish Kumar et al. have reported the study of FASnI3 based solar cell and they have achieved PCE of around 19.08%, short circuit current density of 31.20 mA/cm2, fill factor of 33.72% after optimizing various parameters of ETL (TiO2), HTL (Spiro-OMeTAD) and absorber layer (Kumar et al. 2020; Bouich et al. 2021b). Sn (tin) based perovskite solar cells (PSCs) have certain limitations. Tin is easily get oxidized from Sn2+ to Sn4+, leading to self-doping. It has a detrimental effect on its performance. It leads to low PCE and poor performance, so necessary steps are taken to reduce or eliminate this unwanted process called self-doping arises due to oxidation of tin (Liu et al. 2019a; Mohseni et al. 2021). Tin-based perovskite solar cells (PSCs) have a proper optical bandgap (1.2–1.4 eV) which is in the close proximation of Shockley Queisser Limit (≈1.3 eV). This ideal bandgap can be considered as the biggest motive toward the development of Sn-based or Pb-free perovskite solar cells. Tin-based PSCs provide fast crystallization and low defect tolerance. The self-doping process arising due to unwanted oxidation of tin material causes recombination of excitons (electron–hole) in perovskites (Ke et al. 2019; Cao and Yan 2021; Song et al. 2018; Liu et al. 2019b).

In the present simulation work, we have used (FA0.9EA0.1)0.98EDA0.01SnI3 absorber layer, where EAI (ethyl ammonium iodide) helps to match the energy level which improves crystallinity. Ethalammonium (EA) is used to enhance the extraction process of the electron transport layer and hole transport layer (Nishimura et al. 2020). The primary role of hole transporting materials (HTMs) in devices is to collect and transport after holes are injected from a light harvester, allowing for effective electron and hole separation, which is a vital and necessary aspect of the PSCs. Hence, it will reduce the charge carrier recombination. Thereby, increasing the lifetime of charge carriers (electrons and hole) and conclusively will lead to increase in the lifetime of perovskite solar cells (PSCs). (FA0.9EA0.1)0.98EDA0.01SnI3 based PSCs have been examined and analyzed the impact of thickness, defect density of absorber layer with different hole transport materials. Various hole transport materials such as Poly(3,4-ethylenedioxythiophene)-poly(styrene sulfonate)
(PEDOT: PSS), cuprous oxide (Cu$_2$O), Copper(I) iodide (CuI), and copper zinc tin selenide (CZTSe) are investigated using simulation software. Poly(3-hexylthiophene) (PCBM) and C60 are used as an ETL (Electron transport layer) in the device structure. Device simulation is done for FTO/HTM/(FA$_{0.9}$EA$_{0.1}$)$_{0.98}$EDA$_{0.01}$SnI$_3$/IDL/PCBM/C60/Au inverted structure with parameters of each layer using SCAPS-1D and results of four different structures are analyzed under AM1.5G solar spectrum at 1000 W/m$^2$.

2 Device structure and simulation methodology

2.1 Device structure

Four structures having different hole transport material (HTM) is simulated using SCAPS 1-D (ver. 3.3.10) under AM1.5G illumination with an incident light power of 1000 W/m$^2$. This simulation software is developed at the University of Gent, Belgium to scrutinize the performance of the tin-based solar cell. In SCAPS 1-D, all the calculations for simulations are carried out using three fundamental equations: Poisson equation, hole continuity equation, and electron continuity equation (x, y, z). Using SCAPS 1-D, the heterostructure of solar cells can be designed using seven different layers and we can illuminate the device using light and dark environmental conditions (Bag et al. 2020).

This structure is composed of FTO/HTM (30 nm)/(FA$_{0.9}$EA$_{0.1}$)$_{0.98}$EDA$_{0.01}$SnI$_3$ (550 nm)/IDL (5 nm)/PCBM (30 nm)/C60 (30 nm)/Au is shown in the Fig. 1. In this device structure, (FA$_{0.9}$EA$_{0.1}$)$_{0.98}$EDA$_{0.01}$SnI$_3$ is the perovskite absorber layer (PAL), inserted between the hole transport layer (HTL) and the electron transport layer (ETL). Interface defect layer (IDL) is inserted between perovskite absorber layer (PAL) and PCBM interface to consider interface recombination between holes at the energy of valence band (Ev) of the perovskite absorber layer and electrons at energy of conduction band (Ec) of PCBM layer. FTO is used as a front contact and gold (Au) is used as the back contact. Energy Band diagram of four structures having different hole transport material (HTM) can be seen in Fig. 2. Case (a), (b), (c), (d) represents the band diagram of ITO/HTM/(FA$_{0.9}$EA$_{0.1}$)$_{0.98}$EDA$_{0.01}$SnI$_3$/IDL/PCBM/C60/Au structure, where PEDOT:

![Fig. 1 Device configuration of simulated perovskite solar cell](image)
PSS, Cu$_2$O, CuI, and CZTSe act as a hole transport layers (HTLs). ETM and HTM are used to extract the electrons and holes from the absorber layer and they should have high charge carrier mobility.

For proper transport of electrons, the minimum level of the conduction band of the electron transport layer (ETL) must lie below than minimum level of the conduction band of the perovskite layer. Similarly, in the case of hole transport layer, the maximum level of valence band of hole transport layer must lie above that of the perovskite layer (Singh et al. 2021). Out of different HTL, Cu$_2$O is performing better because it has better band alignment with the perovskite layer and back-contact and high charge carrier mobility. However, it is already shown in the literature that Cu$_2$O can be easily fabricated using low-temperature solution method.

### 2.2 SCAPS simulation methodology

SCAPS (Solar Cell Capacitance Simulator) is a one-dimensional simulation tool for solar cells, which is capable to replicate the features of thin-film solar cells ("Experimental et al. (1–x) S2-based solar cells." 2019; Punetha et al. 2019). Various parameters have been used to perform this research work and they are obtained from various experimental and theoretical research papers. These parameters are summarized in Table 1. The thickness of absorber layer is optimized at 550 nm whereas the thickness of ETL and HTL is best suited at 30 nm. The bandgap of (FA$_{0.9}$EA$_{0.1}$)$_{0.98}$EDA$_{0.01}$SnI$_3$ is 1.42 eV. The total defect density is set at $1 \times 10^{14}$ cm$^{-3}$. As we increase the defect density, the overall efficiency of the device reduces. All the other parameters of HTL, ETL, and perovskite absorber layer are given in Tables 1 and 2.
Table 1  Basic parameters of each layer of the perovskite solar cell (Nishimura et al. 2020; Bag et al. 2020; Singh et al. 2021; Minemoto et al. 2020; Ahmed et al. 2021)

| Parameters                        | Cu$_2$O | (FA$_{0.9}$EA$_{0.1}$)$_{0.98}$EDA$_{0.02}$SnI$_3$ | IDL | PCBM | C60 |
|-----------------------------------|---------|---------------------------------|-----|------|-----|
| Thickness (µm)                    | 0.03    | 0.550                           | 0.005 | 0.03 | 0.03 |
| Bandgap (eV)                      | 2.17    | 1.42                            | 1.07 | 2.1  | 1.7  |
| Electron affinity (eV)            | 3.2     | 3.67                            | 4.0  | 3.9  | 3.9  |
| Dielectric permittivity (relative)| 7.1     | 8.2                             | 8.2  | 3.9  | 4.2  |
| CB effective density of states (1/cm$^3$) | $2.5 \times 10^{18}$ | $1 \times 10^{18}$ | $2.2 \times 10^{18}$ | $2.5 \times 10^{21}$ | $8 \times 10^{19}$ |
| VB effective density of states (1/cm$^3$) | $1.8 \times 10^{18}$ | $1 \times 10^{18}$ | $1.8 \times 10^{19}$ | $2.5 \times 10^{21}$ | $8 \times 10^{19}$ |
| Electron thermal velocity (cm/s)  | $1 \times 10^7$ | $1 \times 10^7$ | $1 \times 10^7$ | $1 \times 10^7$ | $1 \times 10^7$ |
| Hole thermal velocity (cm/s)      | $1 \times 10^7$ | $1 \times 10^7$ | $1 \times 10^7$ | $1 \times 10^7$ | $1 \times 10^7$ |
| Electron mobility (cm$^2$/Vs)     | $2 \times 10^2$ | $9.74 \times 10^2$ | $9.27 \times 10^{-3}$ | $2 \times 10^{-2}$ | $8 \times 10^{-2}$ |
| Hole mobility (cm$^2$/Vs)         | $8 \times 10^2$ | $2.13 \times 10^2$ | $9.27 \times 10^{-3}$ | $2 \times 10^{-2}$ | $3.5 \times 10^{-3}$ |
| Shallow uniform donor density ND (1/cm$^3$) | 0 | $5.48 \times 10^{15}$ | $1 \times 10^{13}$ | $2.93 \times 10^{17}$ | $2.6 \times 10^{18}$ |
| Shallow uniform acceptor density NA (1/cm$^3$) | $9 \times 10^{21}$ | 0 | 0 | 0 | 0 |
| Capture cross section electrons (cm$^2$) and capture cross section holes (cm$^2$) | $2 \times 10^{-14}$ | $2 \times 10^{-14}$ | $2 \times 10^{-14}$ | $2 \times 10^{-14}$ | $2 \times 10^{-14}$ |
| Energy level with respect to Reference (eV) | 0.9 | 0.7 | 0.53 | 1.050 | 0.85 |
| Total defect N$_t$ (1/cm$^3$)     | $1 \times 10^{15}$ | $1 \times 10^{14}$ | $2.5 \times 10^{19}$ | $1 \times 10^{15}$ | $1 \times 10^{15}$ |
2.3 Results and discussion

In this section, we analyze the four structures with different hole transport materials (HTMs) to understand the behavior of solar cells. In the simulation, we worked on how some fundamental parameters of photovoltaic like defect density, operating temperature, the thickness of absorber layer, and bandgap of four different hole transport material influence the performance of the device.

2.4 Comparative study of different HTM for the same thickness of absorber layer and defect scenario

In this subsection, we have inspected with optimization of hole transport materials i.e., PEDOT: PSS, Cu2O, Cul, CZTSe. We have simulated these hole transport materials to choose the best-suited HTM and determine its optimum thickness. Tables 1 and 2 show the various parameters of HTM. Out of four HTM, Cu2O provides the maximum power conversion efficiency as compared to other HTMs. It has the highest charge carrier mobility due to which more carriers are extracted and more current is produced. From Fig. 2, it is also shown that it has better band alignment with the absorber layer. After simulating perovskite solar cells with HTMs, Cu2O gives the best performance parameters with the highest power conversion efficiency of 18.78%.

2.5 Analysis of HTMs with the variation of thickness of absorber layer

To observe the effect of absorber layer thickness on the solar cell, we have varied the thickness of (FA0.9EA0.1)0.98EDA0.01SnI3 from 150 to 550 nm keeping all other

| Parameters                      | PEDOT: PSS | Cul | CZTSe |
|---------------------------------|------------|-----|-------|
| Thickness (µm)                  | 0.03       | 0.03| 0.03  |
| Bandgap (eV)                    | 1.6        | 2.98| 1.4   |
| Electron affinity (eV)          | 3.5        | 2.1 | 4.1   |
| Dielectric permittivity (relative) | 3.0        | 6.5 | 9.0   |
| CB effective density of states (1/cm³) | 1×10²²   | 2.8×10¹⁹ | 2.2×10¹⁸ |
| VB effective density of states (1/cm³) | 1×10²²   | 1×10⁹  | 1.8×10⁹ |
| Electron thermal velocity (cm/s) | 1×10⁷     | 1×10⁷ | 1×10⁷ |
| Hole thermal velocity (cm/s)     | 1×10⁷     | 1×10⁷ | 1×10⁷ |
| Electron mobility (cm²/Vs)       | 4.5×10⁻⁴  | 1.7×10⁻⁴| 1×10² |
| Hole mobility (cm²/Vs)           | 9.9×10⁻⁵  | 2.0×10⁻⁴| 12.5  |
| Shallow uniform donor density ND (1/cm³) | 0        | 0    | 0     |
| Shallow uniform acceptor density NA (1/cm³) | 1×10²⁰ | 1×10¹⁸ | 1×10¹⁹ |
| Capture cross section electrons (cm²) and capture cross section holes (cm²) | 2×10⁻¹⁴ | 2×10⁻¹⁴ | 2×10⁻¹⁴ |
| Energy level with respect to Reference (eV) | 0.9       | 0.9  | 0.9   |
| Total defect Nt (1/cm³)          | 1×10¹⁵    | 1×10¹⁵| 1×10¹⁵|
parameters same. The results are shown in Fig. 3. When a thin layer is used, low photocurrent is produced which results due to less absorption, however, extraction is high. Power Conversion Efficiency is increases with the thickness of perovskite absorber layer because more material is exposed to sunlight and therefore more energy will be absorbed in this layer (Zhou et al. 2018). As a result, more electron–hole pairs are created with enhanced mobility. We can also see the decrease in fill factor with the increase in the thickness of the absorber layer. This is mainly due to the internal recombination inside the perovskite material that is generated due to electron and hole charge carriers, which do not permit an adequate period for charge carriers to develop conduction band at perovskite material (Hasan et al. 2020). The tin-based absorber layer is an excellent absorber material to achieve high power conversion efficiency at a low cost. From testing results, it is observed that on increasing the absorber thickness (t), Voc, Jsc, and PCE increases whereas FF decreases. The calibrated polynomial relation is as follows:

\[
Voc = 0.108 + 0.00631t - 3.53 \times 10^{-5}t^2 + 8.72 \times 10^{-8}t^3
\] (1)

\[
Jsc = 5 + 0.12t - 0.0002t + 1.2t^2 \times 10^{-7}t^3
\] (2)

\[
FF = 75.8 - 0.08t + 0.00145t^2 - 7.136 \times 10^{-6}t^3
\] (3)

\[
PCE = 2.03 - 2.8 \times 10^{-4}t + 5.8 \times 10^{-4}t^2 - 3.13 \times 10^{-6}t^3
\] (4)

Fig. 3 Variation in the absorber thickness with respect to a Open circuit voltage, b Short circuit current density, c Fill factor, d Power conversion efficiency, keeping the same thickness of ETL and HTL.
2.6 Effect of variation in defect density of absorber layer on perovskite solar cell

The defect density is considered as one of the significant parameters of the individual layer. It plays an important role in the performance of the solar cell as it increases the recombination center in the layer. The Shockley–Read–Hall (SRH) recombination model has been employed to study the effect of defect density of the absorber layer on the performance of solar cells as given in following equation (Singh et al. 2021).

\[
R_{SRH} = \frac{np - n_i^2}{\tau_p(n + n_i) + \tau_n(p + p_i)}
\]

(5)

where \( R_{SRH} = \) Shockley–Read–Hall recombination rate, \( n \) and \( p \) = Electron, hole concentration, \( \tau_{n,p}, \sigma_{n,p} \) = lifetime of hole and electron.

The initial defect density of the perovskite layer is considered as \( 10^{16} \) cm\(^{-3} \). Then, we started decreasing it below \( 10^{16} \)–\( 10^{14} \) cm\(^{-3} \). We saw that power conversion efficiency starts increasing with decreasing defect density. It has been observed that if defect density of absorber layer is varied from \( 10^{14} \) to \( 10^{19} \) as shown in Fig. 4. The Voc of Cu\(_2\)O has been
decreased from 0.88 to 0.52 V, Jsc varies from 27.24 mA/cm² to 14.71 mA/cm², Fill Factor varies from 77.93 to 58.23%, and efficiency (η%) varies from 18.78 to 4.51%.

Increase in defect density of the absorber layer will create more recombination centers within the absorber layer due to which more carriers are getting recombined within the absorber layer (Liu et al. 2019a). Also, as the defect density of the absorber layer increases, it will reduce the lifetime of carriers because they are recombined inside the absorber layer and no more carriers are left for extraction which in turn reduces the overall device performance of solar cells as per the Eq. (5) and Eq. (6). Moreover, with the increase in defect density, recombination centers also increase which decreases the shunt resistance of the device which in turn reduces the open-circuit voltage (Voc) (Cao and Yan 2021). Hence, can conclude from the above analysis that for better device performance of the solar cell, the numeric value for defect density of the perovskite layers should be in the order of ~ $1 \times 10^{14}$ cm$^{-3}$ as with the increase in this parameter, the photovoltaic performance has been reduced.

2.7 Effect of operating temperature on the performance of perovskite solar cell

There is a need to understand the effect of operating temperature on the performance of the solar cell. Generally, solar cells are installed in the outer environment where solar panels are continuously illuminated with sunlight. Due to this continuous illumination, it will increase the cell temperature to greater than the room temperature. We have tried to investigate the effect of variation in operating temperature on the performance of the solar cell. The temperature is varied from 200 to 500 K. It has been observed that Voc has been reduced from 1.03 to 0.38 V, Jsc reduces from 27.50 to 26.42 mA/cm², FF varies from 80.74 to 57.82% and power conversion efficiency varies from 22.95 to 5.86% for Cu$_2$O. At higher temperatures, the bandgap reduces due to which more recombination of excitons (electrons and holes) will take place which will further result in the reduction of Voc (Song et al. 2018). Due to an increase in temperature, defects also increase, which will cause reduction in FF and PCE of the device. The results for device ITO/Cu$_2$O/ (FA$_{0.9}$EA$_{0.1}$)$_{0.98}$EDA$_{0.01}$SnI$_3$/IDL/PCBM/C60/Au are shown in Fig. 5.

2.8 J–V and Quantum efficiency

Current density–voltage characteristics (J–V) and Quantum efficiency curves are very imperative for the analysis of solar cell performance. For each device structure having PEDOT: PSS, Cu$_2$O, CuI, CZTSe hole transport materials, the J-V Characteristics, and quantum efficiency are shown in Fig. 6. (FA$_{0.9}$EA$_{0.1}$)$_{0.98}$EDA$_{0.01}$SnI$_3$ based perovskites have a very narrow bandgap. So absorption shifts towards the near infrared region (NIR) (Teimouri and Mohammadpour 2018; Lin et al. 2018; Dixit et al. 2019). Here quantum efficiency curves are covering the whole visible spectrum (400–750 nm) of solar radiation. By analyzing the QE curve, broad absorption maximum of up to 99% with Cu$_2$O has been achieved in this simulation work.

The general structure of tin-based perovskite solar cells consists of (FA$_{0.9}$EA$_{0.1}$)$_{0.98}$EDA$_{0.01}$SnI$_3$ absorber layer. Various compositions of the absorber layer have been simulated. (FA$_{1-x}$EA$_x$)$_{0.98}$EDA$_{0.01}$ SnI$_3$ perovskite with x = 0.1, 0.2, 0.3, 0.4 are taken for deciding the best composition for perovskite layer. Table 3 shows that at x = 0.1, we have reported the maximum efficiency of 18.78.
In perovskite photovoltaic, hole transport layers (HTLs) are not only important for device performance; they also affect total flexibility, cost, and the best tandem solar cell applications. Table 4 shows the optimized parameters of solar cells with four different hole transport materials.

**Fig. 5** The behavior of a Open circuit voltage, b Short circuit current density, c Fill factor, d Power conversion efficiency in variation with the operating temperature of perovskite solar cell.

**Fig. 6** a J–V Characteristics of Perovskite solar cell, b Percentage of quantum efficiency with variation in wavelength.

In perovskite photovoltaic, hole transport layers (HTLs) are not only important for device performance; they also affect total flexibility, cost, and the best tandem solar cell applications. Table 4 shows the optimized parameters of solar cells with four different hole transport materials.
Table 3  Different composition of the perovskite absorber layer

| FA\(_{1-x}\)EA\(_x\) | Voc (V) | Jsc (mA/cm\(^2\)) | FF (%) | PCE (%) |
|---------------------|---------|-------------------|--------|---------|
| FA\(_{0.9}\)EA\(_{0.1}\) | 0.8851  | 27.24             | 77.91  | 18.78   |
| FA\(_{0.8}\)EA\(_{0.2}\) | 0.9141  | 26.17             | 78.07  | 18.68   |
| FA\(_{0.7}\)EA\(_{0.3}\) | 0.9336  | 25.66             | 78.01  | 18.69   |
| FA\(_{0.6}\)EA\(_{0.4}\) | 0.9434  | 25.23             | 78.01  | 18.57   |

Table 4  Performance parameters of perovskite solar cell with different HTMs

| HTMs         | Voc (V) | Jsc (mA/cm\(^2\)) | FF (%) | PCE (%) | Reference                  |
|--------------|---------|-------------------|--------|---------|-----------------------------|
| PEDOT: PSS   | 0.8877  | 23.61             | 76.82  | 16.10   | This Work                   |
| CuI          | 0.8889  | 26.87             | 77.13  | 18.42   | This Work                   |
| CZTS\(_{e}\) | 0.8813  | 22.66             | 77.56  | 15.49   | This Work                   |
| Cu\(_{2}\)O  | 0.8851  | 27.24             | 77.91  | 18.78   | This Work                   |
| PEDOT: PSS   | 0.8400  | 20.32             | 78.00  | 13.24   | Nishimura et al. 2020       |
| Cu\(_{2}\)O  | 1.340   | 15.55             | 82.73  | 18.01   | Singh et al. 2021          |
| CuI          | 1.050   | 15.55             | 81.23  | 13.90   | Singh et al. 2021          |
| PEDOT: PSS   | 0.890   | 22.79             | 65.28  | 13.35   | Pathak and Pandey 2020      |

Fig. 7  J–V and QE-Wavelength curves obtained for both simulation and experimental work

Figure 7 shows the comparison between the experimental (Bouich et al. 2021b) and simulated results. It is shown from the figure that J-V and QE curves which are obtained for both experimental and simulated results are somewhat identical to each other.

3 Conclusion

In this study, we have optimized the performance of lead-free perovskite solar cell for different HTL. This research work comprises the device simulation of lead-free perovskite solar cell. It is obtained from the simulation results, that Cu\(_{2}\)O as HTL shows higher PCE
as compared to PEDOT: PSS, CuI, CZTSe based perovskite structure. It has been reported that Cu₂O has a better band alignment with the absorber layer. By optimization the device parameters we have achieved Voc = 0.8851 V, Jsc = 27.24 mA/cm², FF = 77.91%, and PCE = 18.78% for FTO/Cu₂O/(FA₀.⁹EA₀.¹)₀.₉₈EDA₀.₀₁SnI₃/IDL/PCBM/C₆₀/Au device structure. The defect density of the perovskite absorber layer is found to be 1 × 10¹⁴ cm⁻³ for better performance. A further effect of operating temperature has also been studied to investigate the performance of tin-based perovskite solar cells and the optimized results have been achieved at 300 K. With the increase in temperature, the device starts degrading due to the infusion of certain defects which will cause instability issues. These results represent the potential of (FA₀.⁹EA₀.¹)₀.₉₈EDA₀.₀₁SnI₃ based solar cell (lead free) which can provide support to the research community to design more stable and environment friendly solar cell.

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Declarations

Conflict of interest The authors have not disclosed any conflict of interest.

References

Ahmed, S., Jannat, F., Khan, M.A.K., Alim, M.A.: Numerical development of eco-friendly Cs₂TiBr₆ based perovskite solar cell with all-inorganic charge transport materials via SCAPS-1D. Optik 225, 165765 (2021)

Bag, A., Radhakrishnan, R., Nekovei, R., Jeyakumar, R.: Effect of absorber layer, hole transport layer thicknesses, and its doping density on the performance of perovskite solar cells by device simulation. Sol. Energy 196, 177–182 (2020)

Bouich, A., Hartiti, B., Ullah, S., Ullah, H., Touhami, M.E., Santos, D.M.F., Mari, B.: Experimental, theoretical, and numerical simulation of the performance of CuInₓGa (1–x) S₂-based solar cells. Optik 183, 137–147 (2019)

Bouich, A., Mari, B., Atourki, L., Ullah, S., Touhami, M.E.: Shedding light on the effect of diethyl ether antisolvent on the growth of (CH₃NH₃) PbI₃ thin films. JOM 73(2), 551–557 (2021a)

Bouich, A., Ullah, S., Mari, B., Atourki, L., Touhami, M.E.: One-step synthesis of FA₁–xGAXPbI₃ perovskites thin film with enhanced stability of alpha (α) phase. Mater. Chem. Phys. 258, 123973 (2021b)

Cao, J., Yan, F.: Recent progress in tin-based perovskite solar cells. Energy Environ. Sci. 14(3), 1286–1325 (2021)

Chang, X., Fang, J., Fan, Y., Luo, T., Su, H., Zhang, Y., Lu, J., et al.: Printable CsPbI₃ perovskite solar cells with PCE of 19% via an additive strategy. Adv. Mater. 32(40), 2001243 (2020)

Chen, K., Jin, W., Zhang, Y., Yang, T., Reiss, P., Zhong, Q., Bach, U., et al.: High efficiency mesoscopic solar cells using CsPbI₃ perovskite quantum dots enabled by chemical interface engineering. J. Am. Chem. Soc. 142(8), 3775–3783 (2020)

Dixit, H., Punetha, D., Pandey, S.K.: Improvement in performance of lead free inverted perovskite solar cell by optimization of solar parameters. Optik 179, 969–976 (2019)

Dixit, H., Punetha, D., & Pandey, S. K. Comparative study and analysis of different perovskite solar cells with inverted architecture. In computational Mathematics, Nanoelectronics, and Astrophysics: CMNA 2018, Indore, India, pp. 125–135. Springer, Singapore (2021)

Haase, F., Hollemann, C., Schäfer, S., Merkle, A., Rienäcker, M., Krügener, J., Peibst, R.: Laser contact openings for local poly-Si-metal contacts enabling 26.1%-efficient POLO-IBC solar cells. Sol. Energy Mater. Sol. Cells 186, 184–193 (2018)

Hasan, S.A.U., Lee, D.S., Im, S.H., Hong, K.H.: Present status and research prospects of tin-based perovskite solar cells. Solar RRL 4(2), 1900310 (2020)
Jiang, Q., Zhao, Y., Zhang, X., Yang, X., Chen, Y., Chu, Z., You, J.: Surface passivation of perovskite film for efficient solar cells. Nat. Photonics 13(7), 460–466 (2019)

Ke, W., Stoumpos, C.C., Kanatzidis, M.G.: “Unleaded” perovskites: status quo and future prospects of tin-based perovskite solar cells. Adv. Mater. 31(47), 1803230 (2019)

Kumar, M., Raj, A., Kumar, A., Anshul, A.: An optimized lead-free formamidinium Sn-based perovskite solar cell design for high power conversion efficiency by SCAPS simulation. Opt. Mater. 108, 110213 (2020)

Lin, J., Lai, M., Dou, L., Kley, C.S., Chen, H., Peng, F., Yang, P.: Thermochromic halide perovskite solar cells. Nat. Mater. 17(3), 261–267 (2018)

Liu, W.W., Wu, T.H., Liu, M.C., Niu, W.J., Chueh, Y.L.: Recent challenges in perovskite solar cells toward enhanced stability, less toxicity, and large-area mass production. Adv. Mater. Interfaces 6(9), 1801758 (2019a)

Liu, T., Zhao, X., Li, J., Liu, Z., Liscio, F., Milita, S., Fenwick, O.: Enhanced control of self-doping in halide perovskites for improved thermoelectric performance. Nat. Commun. 10(1), 1–9 (2019b)

Minemoto, T., Kawano, Y., Nishimura, T., Shen, Q., Yoshino, K., Ikubono, S., Chantada, J.: Theoretical analysis of band alignment at back junction in Sn–Ge perovskite solar cells with inverted pin structure. Sol. Energy Mater. Sol. Cells 206, 110268 (2020)

Mohseni, H.R., Dehghanipour, M., Dehghan, N., Tamaddon, F., Ahmadi, M., Sabet, M., Behjat, A.J.S.E.: Enhancement of the photovoltaic performance and the stability of perovskite solar cells via the modification of electron transport layers with reduced graphene oxide/polyaniline composite. Sol. Energy 213, 59–66 (2021)

Nishimura, K., Kamarudin, M.A., Hirotani, D., Hamada, K., Shen, Q., Ikubono, S., Hayase, S.: Lead-free tin-halide perovskite solar cells with 13% efficiency. Nano Energy 74, 104858 (2020)

Pathak, C., Pandey, S.K.: Design, performance, and defect density analysis of efficient eco-friendly perovskite solar cell. IEEE Trans. Electron Devices 67(7), 2837–2843 (2020)

Punetha, D., Pandey, S.K.: Enhancement and optimization in sensing characteristics of ammonia gas sensor based on light assisted nanostructured WO3 thin film. IEEE Sens. J. 20(24), 14617–14623 (2020)

Punetha, D., Dixit, H., Pandey, S.K.: Modeling and analysis of an Ni:ZnO-based Schottky pattern for NO2 detection. J. Comput. Electron. 18(1), 300–307 (2019)

Punetha, D., Kar, M., Pandey, S.K.: A new type low-cost, flexible and wearable tertiary nanocomposite sensor for room temperature hydrogen gas sensing. Sci. Rep. 10(1), 1–11 (2020)

Sahli, F., Werner, J., Kamino, B.A., Bräuning, M., Monnard, R., Paviet-Salomon, B., Balloffet, C.: Fully textured monolithic perovskite/silicon tandem solar cells with 25.2% power conversion efficiency. Nat. Mater. 17(9), 820–826 (2018)

Singh, N., Agarwal, A., Agarwal, M.: Numerical simulation of highly efficient lead-free perovskite layers for the application of all-perovskite multi-junction solar cell. Superlattices Microstruct. 149, 106750 (2021)

Song, T.B., Yokoyama, T., Logsdon, J., Wasielewski, M.R., Aramaki, S., Kanatzidis, M.G.: Piperazine suppresses self-doping in CsSnI₃ perovskite solar cells. ACS Appl. Energy Mater. 1(8), 4221–4226 (2018)

Teimouri, R., Mohammadpour, R.: Potential application of CuSbS₂ as the hole transport material in perovskite solar cell: a simulation study. Superlattices Microstruct. 118, 116–122 (2018)

Yang, W.S., Park, B.W., Jung, E.H., Jeon, N.J., Kim, Y.C., Lee, D.U., Seok, S.I.: Iodide management in formamidinium-lead-halide–based perovskite layers for efficient solar cells. Science 356, 1376–1379 (2017)

Zhou, D., Zhou, T., Tian, Y., Zhu, X., Tu, Y.: Perovskite-based solar cells: materials, methods, and future perspectives. J. Nanomater. 2018, 1–16 (2018)

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