Attainment of Stable (FTO/ZnO/CdS/CH3NH3SnI3/GaAs/Au) Perovskite Solar Cell With Above 23% Photovoltaic Performance Using Solar Capacitance Simulator

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Research Article

Keywords: Perovskites, Solar Cells, Absorber layer, Current Density, Efficiency  
PACS codes: 74.25.-q, 74.25.F-, 74.72.-h, 74.81.Bd

Posted Date: August 10th, 2021

DOI: https://doi.org/10.21203/rs.3.rs-731428/v1

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Attainment of Stable (FTO/ZnO/CdS/CH₃NH₃SnI₃/GaAs/Au) Perovskite Solar Cell with above 23% Photovoltaic Performance Using Solar Capacitance Simulator

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Abstract

Solar energy is found to be low cost and abundant of all available energy resources and needs exploration of highly efficient devices for global energy requirements. We have investigated methyl ammonium tin halide (CH₃NH₃SnI₃)-based perovskite solar cells (PSCs) for optimized device performance using solar capacitance simulator SCAPS-1D software. This study is a step forward towards availability of stable and non-toxic solar cells. We explored all necessary parameters such as metal work functions, thickness of absorber and buffer layers, charge carrier’s mobility and defect density for improved device performance. Calculations revealed that for the best efficiency of device the maximum thickness of the perovskite absorber layer must be 4.2 μm. Furthermore, optimized thickness values of (ZnO=0.01 μm) as electron transport layer (ETL), GaAs as hole transport layer (HTL=3.02 μm) and (CdS=10 nm) and buffer layer have provided power conversion efficiency (PCE) of 23.53%. Variation of open circuit voltage (Vₜₐₓ), Short circuit current (Iₘₜₐₓ), Fill Factor (FF%) and quantum efficiency against thickness of all layers in FTO/ZnO/CdS/CH₃NH₃SnI₃/GaAs/Au compositions have been critically explored and reported. Interface defects and defect density in different inserted layers
have also been reported in this study as they can play a crucial for the device performance. Insertion of ZnO layer and CdS buffer layers have shown improved device performance and PCE. Current investigations may prove to be useful for designing and fabrication of climate friendly, non-toxic and highly efficient solar cells.

Key words: Perovskites, Solar Cells, Absorber layer, Current Density, Efficiency
PACS codes: 74.25.-q, 74.25. F-, 74.72.-h, 74.81.Bd.

1. Introduction

Nowadays energy consumption has been increased steadily with civilization development, and in order to keep up with the pace of the development of modern society in the near future, the energy or power consumption will be further increased which might result a crisis situation. In recent years, Inorganic and organo-halides solar cells with perovskite absorber materials have drawn tremendous considerations in the photovoltaic community because of their outstanding photoelectric performance, high electrical parameters such as current density and quantum efficiency and low manufacturing cost [1-3]. The physical, mechanical and optoelectronic properties of perovskite materials are recommended for the PV application. Researchers have analyzed some of these properties by using first-principle method with density functional theory (DFT) [4, 5]. A typical perovskite solar cell employed organic-inorganic halide material as active material [6, 7]. Although, these types of materials exhibit efficiency of more than 20% but, there are two main concerns associated with it. First, these kinds of materials consist of organic cation which create instability and thereby suppressing the life time of the perovskite material and second is the toxicity of lead (Pb) which is highly hazardous to our environment [8]. On the other hand, the energy band gap of inorganic-halide perovskite (Sn, Ag, Sb, Bi, Cu) based solar cells is more than 2eV which is less suitable for the PV application [9, 10]. Furthermore, some other challenges are also linked with such perovskite materials. For example, the open-circuit voltage of Sn$^{2+}$ cation and Sb is quite low, oxidation of Ge$^{2+}$ cation makes it unstable, Bi has poor charge transport ability; Cu has inferior PV properties etc. To date, the maximum PCE of perovskite based solar cell is recorded 25.2% which is quite greater than the efficiency recorded 3.8% in 2009 [11, 12]. This tremendous achievement has brought perovskite solar cells in photovoltaic market as compare to Si-based solar cells [13]. However, some hole-transporting material materials (HTM) like Spiro-OMETAD has restricted the perovskite absorber materials based solar cells to market because of their heavy manufacturing cost and suppression of long time
Scientists in the field of perovskite solar cells have obtained better advancement of high mobility, absorption co-efficient and tunable band gap of the absorber layer but still some main problems like stability degradation, toxic nature of lead, hysteresis, high cost and high-power conversion efficiency are challenged. So, there is inexorable need to optimize the parameters of perovskite solar cells for better performance at low manufacturing cost. An active way for achieving the required results is to optimized performance of Perovskite solar cells, typically Organo-Halide Perovskite absorber materials e.g., CH$_3$NH$_3$XY$_3$ (X=Pb, Sn, Ge & Y= Cl, Br, I) in which the major focus is to reduce toxicity and enhance stability. Several compositional and structural derivatives of perovskite family including layered Ruddlesden-Popper perovskites and double perovskites are needed to be explored on the basis of best available computational and experimental resources. Hui-Jing Du et.al, studied the electrical parameters and device structure stability of CH$_3$NH$_3$SnI$_3$ perovskite absorber layer by simulations. The electrical parameters such as $V_{oc}$, $J_{sc}$, FF and PCE was found to be 0.92V, 31.59 mA/cm$^2$, 79.99% and 23.36% respectively. Furthermore, CH$_3$NH$_3$SnI$_3$ perovskite absorber material was found more efficient than CH$_3$NH$_3$PbI$_3$ due to non-toxicity and Sn$^{+2}$ stability of Sn element in CH$_3$NH$_3$SnI$_3$ structure [16]. Nacereddine Lakhdar.et.al, calculated the optimized PCE of 13.5% for CH$_3$NH$_3$GeI$_3$ based perovskite solar cell by inserting $C_60$ as ETM layer through SCAPS-1D [17]. Hima et al. reported the maximum and optimized PCE of 18.16% for CH$_3$NH$_3$PbI$_3$ solar cell and 9.56% for CH$_3$NH$_3$SnI$_3$ solar cell by using SILVACO ATLAS simulation software [18]. Abdelaziz et al. have reported the influence of defect density, layer thickness and doping concentration in iodide (HC(NH$_2$)$_2$SnI$_3$ – FASnI$_3$) based PSC through SCAPS simulation. The maximum PCE of 14.03% of the optimized device were reported with $V_{oc}$ of 0.92 V, $J_{sc}$ of 22.65 mA/cm$^2$ and FF of 67.74% [19] K.D. Jayan and made a comprehensive device analysis for a variety of electron and hole transport layers along with variation in metal contact using CH$_3$NH$_3$SnI$_3$ perovskite as absorber material and proposed thermodynamic stability of tin based solar cells. Maximum device efficiency of 25.05% was achieved in Glass/FTO/PCBM/MA$\text{SnI}_3$/CuI/Au configuration [20]. Liu et al. studied the effect of absorber layer thickness, charge mobility and defect density on planar PSC with efficiency over 20% using AMPS-1D [21]. Yichuan et.al studied about carrier concentration and carrier mobility of natively textured surface of gallium-doped zinc oxide (GZO) films- based perovskite solar cell with maximum PCE of 21.132% [22]. In lead free MAGeI$_3$ based perovskite solar cell
showed better combination of device parameters with 18.03% efficiency in ITO/ZnO/MAGeI$_3$/Spiro-OmeTAD/Au configuration [23]. CH$_3$NH$_3$SnI$_3$ is a lead-free inorganic perovskite material. This material is suitable for light absorption layer due to its low energy gap of 1.35 eV, high absorption coefficient and high hole mobility of $10^4$ cm$^{-1}$ and 585 cm$^2$/ V$^{-1}$s$^{-1}$ respectively at room temperature. Therefore, Sn$^{2+}$ is highly recommended in halide perovskite solar cells because of their excellent photoelectric performance and also Sn$^{2+}$ is a non-toxic cation as compared to Pb$^{2+}$ions [24-26].

In our current research work, CH$_3$NH$_3$SnI$_3$ based PSCs have been studied and the influences of temperature, thickness of absorbing different layers i.e., absorber, HTL, ETL, defect density and interface defects, carrier recombination and energy band gaps have been reported for optimum device performance. The fundamental objective of our current research work is to optimize all possible characteristic parameters of PSCs precisely in such a way that we can get a high PCE of the device and reduce the fabrication cost.

2. Device Simulation

The device modeling and optimization of PSC can be done by using SCAPS-1D software version (3.3.08) [27]. It was developed by university of Gent, Belgium in which the algorithm is based on three different coupled partial differential-equations (PDEs), namely, Poisson’s equation, continuity equation for holes and electrons, which are given below;

\[
\frac{\partial^2 \Psi}{\partial x^2} = -\frac{\partial E}{\partial x} = -\frac{\rho}{\varepsilon_s} = -\frac{q}{\varepsilon_s}[p-n + N_d^+ - N_a^- + N_{def}] \tag{1}
\]

Where $\Psi$ is electrostatic potentiality, $\varepsilon_s$ is static relative permittivity, $q$ is the charge, e and n are the respective electrons and holes, $N_d^+$ is density of donor, $N_a^-$ is density of acceptor and $N_{def}$ is the defect density of both donor and acceptor. The carrier continuity equation in device may be represented as given below;

\[-\frac{\partial j_p}{\partial x} + G - U_p(n, p) = 0 \tag{2}\]

And

\[-\frac{\partial j_n}{\partial x} + G - U_n(n, p) = 0 \tag{3}\]

Here $j_p$ and $j_n$ are the hole and electron current densities, G is carrier generation rate, $U_n$ (n, p) and $U_p$ (n, P) are the recombination rates of electrons and holes respectively. Furthermore, carrier
current density may also be obtained from:

\[ j_p = qn \mu_p E - qD_p \frac{\partial p}{\partial x} \]  \hspace{1cm} (4)

\[ j_n = qn \mu_n E + qD_n \frac{\partial n}{\partial x} \]  \hspace{1cm} (5)

Here q is the charge, \( \mu_p \) and \( \mu_n \) are carrier mobilities, and \( D_p \), \( D_n \) are the diffusion coefficients.

We can find different parameters of a solar cell through simulations such as current density (\( J_{sc} \)), PCE in percentage, fill factor (FF) in percentage and open circuit voltage (\( V_{oc} \)) against various thickness at all temperatures. Moreover, simulations in SCAPS-1D for seven different layers of a solar cell can work both in light and dark environments at various temperatures [32, 33]. The device configuration of the simulated perovskite based solar cell FTO/ZnO/CdS/CH\(_3\)NH\(_3\)SnI\(_3\)/GaAs/Au is consist of CH\(_3\)NH\(_3\)SnI\(_3\) layer which acts like a light harvesting material, inserted between Hole Transport Layer HTL (GaAs) and Buffer Layer (CdS) and Electron Transporting Layer ETL (ZnO). Fluorine doped tin oxide (FTO) is used as front contact and gold (Au) thin layer as back metal contact.

3. Simulation methodology

The architecture model and device structure used for simulated solar cell FTO/ZnO/CdS/CH\(_3\)NH\(_3\)SnI\(_3\)/GaAs/Au is illustrated in Fig. 1. In this configuration, the work functions of Au and FTO have been taken from the literature i.e. 5.1 eV for Au and 4.4 eV for FTO material. The working procedure involving characteristic steps being carried out during optimization and evaluation process of the device are shown in Fig.2. The material parameter for each layer were taken from various literatures for simulations purpose and is shown in table.1. And the thickness of each layer was optimized for maximum output.

The interfacial defect layers CdS/CH\(_3\)NH\(_3\)SnI\(_3\)-Peroskite and CH\(_3\)NH\(_3\)SnI\(_3\)-Peroskite/GaAs were also taken for simulations purpose with parameters shown in table.2. Initially the arbitrary thickness of ZnO layer was set 0.07 \( \mu m \), CH\(_3\)NH\(_3\)SnI\(_3\)-Peroskite layer 0.4 \( \mu m \) and GaAs layer 1 \( \mu m \). The processes of optimizations of layer thickness was obtained by changing the thickness of one layer and keep constant the thickness of other two layers. The maximum PCE was noted for optimized layer thickness. Similarly, the batch parameters setting for each layer thickness was also varied. At first, ZnO layer thickness was varied from 0.010 \( \mu m \) to 4.00 \( \mu m \) and maximum PCE was noted corresponding to optimized layer thickness of ZnO. Then CH\(_3\)NH\(_3\)SnI\(_3\)-Peroskite
layer was varied from 0.200 μm to 5.00 μm and maximum PCE was noted corresponding to optimized layer thickness of CH$_3$NH$_3$SnI$_3$-Peroskite. Keeping constant the layer thickness of ZnO and CH$_3$NH$_3$SnI$_3$-Peroskite layer, the thickness of GaAs was varied from 0.050 μm to 6.000 μm and maximum PCE was noted corresponding to optimized layer thickness [28]. Similarly, keeping constant all the thickness of layers, the thickness of CdS layer was varied from 0.001 μm to 1 μm. Finally, we found the optimized results for FTO/ZnO/CdS/CH$_3$NH$_3$SnI$_3$/GaAs/Au solar cell device against optimized layers thickness values.

4. Results and Discussion

4.1 Optimized electrical parameters of CH$_3$NH$_3$SnI$_3$-based perovskite solar cell

The electrical parameters and characteristic thickness values of all structural layers were delicately examined to achieve optimum device parameters. The energy band alignment diagram of optimized device is shown in Fig. 3. Beyond these values, even a slight variation in the inserted layers parameters may suppress the performance of device. The J-V characteristics of the solar cell are presented in Fig.4. It is observed that at optimized thickness values of ETL/Buffer/Absorber/HTL layers of solar cell the observed open circuit voltage ($V_{oc}$) has been observed to be 0.923 volts, short circuit current density ($J_{sc}$) value was found to be 33.85752 mA/cm$^2$ and an improved 75.38% value of fill factor. These performance results have been attained at optimum parameters of the device.

The overall layout of the maximum device performance for various parameters is represented in Fig.5. The energy band gaps were fine tuned to achieve the values of 1.42eV for GaAs, 1.35eV for CH$_3$NH$_3$SnI$_3$- absorber, 2.44eV for CdS layer and 3.370 eV for ZnO electron transport layer. Fluorine doped Tin Oxide with work function ($\varphi = 4.4$ eV) and Gold (Au) metal contacts ($\varphi = 5.1$ eV) are also specified in the optimized device.

The carrier mobility of the absorber layer has a remarkable effect on the device performance. Low hole mobility causes a high series resistance and thus restrict the current in the device, leading to an undesirable performance. The PCE% for CH$_3$NH$_3$SnI$_3$ perovskite absorber is observed to be increasing for enhanced values of hole and electron mobilities. A more detailed interpretation related to the trade-off between carrier recombination rate and carrier mobility and can be understood as follow. Considering the equation:

$$V_{oc} = \ln \left(\frac{J_{sc}}{J_0} + 1\right) \frac{KT}{q} \quad (6)$$
According to the Einstein equation

$$\frac{\mu}{K_T} = D_{np} (7)$$

A larger mobility ($\mu$) means a larger diffusion coefficient ($D$), a larger reverse saturation current ($J_{oc}$), when temperature ($T$), diffusion length and doping concentration stay constant. A larger mobility may lead to an increased current density and decreased $V_{oc}$, which directly suppressed PCE. This suggests that, for high performance solar cells, a low electron carrier recombination rate is relatively more important than a high electron carrier mobility [29, 30]. The interface defect layers at i.e., GaAs/CH$3$NH$3$SnI$3$, ZnO/CdS and CH$3$NH$3$SnI$3$/CdS interfacial layers have been considered for the simulations of the proposed perovskite solar cells. Numerical simulation has been performed on the defect density at both interfaces from $1.0 \times 10^{10}$ cm$^{-3}$ to $1.0 \times 10^{19}$ cm$^{-3}$. Fig.6 shows the effect of interface defect density versus PCE curves for optimized perovskite solar cell all interface layers. From the graphs, it can be deduced that increasing interface defect densities, the recombination rate also improves which in turn reduces the PCE. The higher defect densities of the interfaces bring more traps and recombination centers, and deteriorate the performance of cells. So, it can be realized from the simulated results that interface defect density of $1 \times 10^{10}$ cm$^{-3}$ is optimum for device simulation. Fig.7 shows the relationship of carrier’s recombination (cm$^{-3}$.s) and diffusion length ($\mu$m) of the optimized solar cell. $G_{eh}$ of $1.346 \times 10^{22}$ cm$^{-3}$.s is found to be maximum at 7.22 $\mu$m. Also, it is clear that with the enhancement of diffusion length, carrier’s recombination also increases and thus will degrade the performance of solar cell [31]. Furthermore SHR recombination and total recombination are approximately equal and are found to be maximum at $9.42 \times 10^{17}$ cm$^{-3}$.s at 7.27 $\mu$m. The quantum efficiency vs wavelength of incident radiations is represented in Fig.8. It illustrates maximum absorption in visible region range of wavelength. The high value of quantum efficiency means better absorption of the light. Degradation in efficiency is noticed in far-infrared region of wavelength. Beyond these limits a suppression in device performance is observed. Quantum efficiency of 23.53 %, current density ($J_{oc}$) of 33.958782 mA/cm$^2$, open circuit voltage ($V_{oc}$) of 0.923 V and Fill Factor (FF) of 75.38 % is observed for the optimized FTO/ZnO/CdS/CH$3$NH$3$SnI$3$/GaAs/Au solar cell.

4.2Effects of ZnO Electron Transport Layer Thickness

The effect of thickness of the electron transport layer (ZnO) on device performance has been studied using SCAPS-1D. It has been observed that as the thickness of ZnO Layer increases from
0.010 μm to 2.000 μm in seven steps, the open circuit voltage ($V_{oc}$), short-circuit current density ($J_{sc}$), Fill Factor (FF) and quantum efficiency (eta%) is slightly reduced and then become constant from 2.00 μm to 4.00 μm. The variation of electrical parameters ($V_{oc}$, $J_{sc}$, FF% and PCE%) versus thickness for ZnO layer correspond to layer thickness is illustrated in Fig. 9. The maximum values of electrical parameters such as efficiency, short-circuit current density, open circuit voltage and Fill Factor were recorded 15.65%, 29.758527 mA/cm$^2$, 0.7572 V and 69.44% respectively at 0.010 μm. It means that the electrical parameters of the organic-inorganic perovskite-based solar cell are not too much affected by electron transport layer (ETL) [32]. This is explained on the basis of the fact that perovskite compound itself could help the generation of charge carriers by photon excitation and ETL layer is just a charge transport layer.

4.3 Effects of CdS Buffer Layer Thickness

The variation of thickness of the CdS (buffer layer) corresponds to different electrical parameters were checked and presented in Fig. 10. The increase of CdS layer thickness reduced all the electrical parameters ($J_{sc}$, $V_{oc}$, Eta% or PCE%) except FF%. The possible reason for the improvement in FF may be the role of CdS layer in reducing the carrier recombination which ultimately increase the area under the voltage versus current density curve. The optimized values for $J_{sc}$, $V_{oc}$, FF%, Eta% were recorded ~31.626980 mA/cm$^2$, 0.9215 V, 61.11% and 17.81% at 10 nm.

4.4 Effects of CH$_3$NH$_3$SnI$_3$ Absorber Layer Thickness

Fig. 11 shows the thickness of the CH$_3$NH$_3$SnI$_3$ (light-absorber layer) for different electrical parameters. The power conversion efficiency (PCE), current density ($J_{sc}$) and open circuit voltage ($V_{oc}$) gradually increases with the increase of layer thickness. The maximum PCE, current density $J_{sc}$ and open circuit voltage $V_{oc}$ were recorded 20.73%, 33.766332 mA/cm$^2$ and 0.7683 V corresponds to optimized light-absorber layer thickness of 4.20 μm. This happens because the enhanced efficiency is due to the increase in the current density as the light-absorber layer thickness is increased. The increase in absorber layer thickness helps in enhancing the carrier generation due to more exposure of the absorber material to light [33-35]. More electron–hole pairs are generated and thereby electron mobility is increased as shown by the increased $J_{sc}$. The only electrical parameter Fill Factor (FF%) initially increases up to 80.26% at 3.40 μm but then gradually decreases as the layer thickness is increased up to 5.0 μm. This can be due to the recombination of the charge carriers and reduction in lifetime of the charge carrier in the
CH$_3$NH$_3$SnI$_3$-perovskite layer [36]. The recorded electrical parameters for various layer thicknesses were rechecked and confirmed.

4.5 Effects of GaAs Hole Transport Layer Thickness

Properties like high efficiency, flexibility and light weight, resistance to UV radiation and moisture and a low temperature coefficient make gallium arsenide (GaAs) more favorable than the ubiquitously-used silicon for solar cells. In this study, GaAs is acting as a hole transport layer in device structure as shown in Fig. 10. The variation of thickness of GaAs layer from 0.050 μm to 6.00 μm has been studied on perovskite solar cell. The maximum power conversion efficiency (PCE) was found to be 15.41% against the optimized thickness of 3.02 μm. The Fill Factor (FF%) gradually increases with the increase of thickness and was found to be maximum up to 72.78% at 0.050 μm while the current density ($J_{sc}$), open circuit voltage ($V_{oc}$) and power conversion efficiency (PCE) initially enhances with the enhancement of thickness up to 3.02 μm but then suppressed as the thickness is further increased up to 6 μm. The behavior of $V_{oc}$, $J_{sc}$, FF% and PCE% can be seen in Fig. 12. All the electrical parameters such as $J_{sc}$, PCE, $V_{oc}$ and FF% correspond to layer thickness of GaAs layer were rechecked and confirmed.

4.6 Effects of Temperature on Optimized CH$_3$NH$_3$SnI$_3$-based Solar Cell

Solar cells are greatly affected by temperature T(K) when exposed to sunlight. It is important to investigate the performance of optimized solar cells as a function of temperature T(K). The temperature dependence electrical parameters of optimized perovskite solar cells have been shown in Fig.13. There is initially increasing trend in the FF% and after 300K there is continuous decrease in its value. Practically, the rise in temperature give rise to carrier creation but, at the same time higher phonon movements and collisions also play dominant role in reduction of FF PCE and $V_{oc}$. For the rise in FF% the possible reason may be higher stability, higher thickness value and reduced recombination rate and lifetimes associated with carriers in CH$_3$NH$_3$SnI$_3$ absorber. A critical review of the results indicates that there is enhancement in the value of current density from 33.0 mA/cm$^2$ to 35.9817 mA/cm$^2$ with rise in temperature up to 340 K. The increase in $J_{sc}$ may be due to the fact that higher temperatures lead to lattice expansion and attenuation of interatomic bonds. Consequently, higher cell temperatures result in a shrinking of the energy band gap, which means more photons are absorbed, which in turn, leads to free charge carriers being produced. That interpreted as a greater flow of electrons (i.e., more current is generated) with low energies (i.e., a drop-in voltage). Therefore, this leads to decreases in
voltage. On the other hand, however, the rise in current leads to a reduction in maximum power, fill factor, as well as the conversion efficiency. The suggested thickness value 4.2µm of CH$_3$NH$_3$SnI$_3$ absorber, help in maintain longer carrier life time and CdS window layer help reducing carrier recombination to some extent which ultimately help in covering more area under J$_{sc}$ Versus V$_{oc}$ curve indicating improved FF%. Slight reduction in V$_{oc}$ may also be attributed to presence of CdS buffer layer which cause parasitic absorption with increasing thickness. The lower wavelength photons are perturbed to reach the absorber layer which ultimately reduce output current, V$_{oc}$ and overall efficiency.

5. Conclusion
In our current study, FTO/ZnO/CdS/CH$_3$NH$_3$SnI$_3$/GaAs/Au perovskite solar cell was systematically optimized and studied for better power conversion efficiency (PCE) and current density (J$_{sc}$) using SCAPS-1D simulation software. The influence of change in layer thickness of CH$_3$NH$_3$SnI$_3$ (Absorber Layer), ZnO (ETM Layer), GaAs (HTM Layer) and CdS (Buffer Layer) on the electrical parameters were optimized at values 4.200 μm, 0.01 μm, 3.200 μm and 0.01 μm respectively with a better power conversion efficiency (PCE), current density, open circuit voltage and Fill Factor of ~23.53%, 33.8575 mA/cm$^2$, 0.9264 V and 74.94% respectively. The PCE of GaAs-HTL and CH$_3$NH$_3$SnI$_3$-absorber increases with the increase of hole and electron mobilities, whereas the PCE of CdS-Buffer and ZnO-ETL suppress with the increase of hole mobility. The effects of interface defect density versus PCE show no effect on efficiency for CH$_3$NH$_3$SnI$_3$/GaAs and ZnO/CdS interfaces. The effect of energy band-gap tuning of individual layer for optimized performance showed improved PCE for energy band-gap values of 1.42eV for GaAs, 1.35eV for CH$_3$NH$_3$SnI$_3$-absorber, 2.44eV for CdS-Buffer and 3.37eV for ZnO-ETL. This may happen due to the stronger recombination of charge carriers at interfaces before being collected. The enhancement of diffusion length increased the carrier’s recombination rate and thus degraded the performance of solar cell. Furthermore, maximum efficient performance of the device is observed in temperature range of 270K – 280K. These results emphasize the need to improve and enhance the research being carried out in sustainable energy sector and particularly in multi-layer organic and inorganic halide solar cells. GaAs hole transport layer in photovoltaics, can potentially lead to light-weight, inexpensive and scalable solar cell manufacturing, ZnO as electron extraction layer in photovoltaic devices carry high mobility and low processing temperature and CH$_3$NH$_3$SnI$_3$ perovskite absorber is environment friendly and
stable. So, combination of all of these three FTO/ZnO/CdS/CH$_3$NH$_3$SnI$_3$/GaAs/Au provides better results to be used to predict the lead-free CH$_3$NH$_3$SnI$_3$ perovskite solar cell device in terms of better power conversion efficiency (PCE) value with improved electrical parameters.

6. Acknowledgement
The authors are thankful to the Marc. Burgelman and his team at the electronics and Information Systems (ELIS), University of Gent, Belgium for provision of access to SCAPS software.

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Fig. 1

- FTO (Front Contact Layer)
- ZnO (ETM Layer)
- CdS (Buffer Layer)
- CH$_3$NH$_3$SnI$_3$ (Absorber)
- GaAs (HTM Layer)
- Au (Back Contact Layer)
Launch SCAPS
Click set problems
Give input parameters
Set working conditions
Specify the actions to be measured
Run the program

Fig. 2
FTO/ZnO/CdS/CH$_3$NH$_3$SnI$_3$/GaAs/Au

Optimized solar cell with PCE = 23.53%

$V_{oc} = 0.926$ V
$J_{sc} = 33.8575$ mA/cm$^2$
FF = 74.94%

Fig.4
Fig. 5
Fig. 6
Fig. 7

Optimized solar cell performance

- Generation rates (cm$^{-3}$s$^{-1}$)
  - Geh (cm$^{-3}$s$^{-1}$)

Recombination rates (cm$^{-3}$s$^{-1}$)
- Total recombination (cm$^{-3}$s$^{-1}$)
  - SRH recombination (cm$^{-3}$s$^{-1}$)
Quantum Efficiency QE (%) vs. Wavelength (nm)

- Optimized Solar Cell:
  FTO/ZnO/CdS/CH$_3$NH$_3$SnI$_3$/GaAs/Au

Visible spectrum of Sunlight

Fig. 8
ZnO (ETM)

- **Eta (%) vs X**
- **FF (%) vs X**
- **J_{sc} (mA/cm^2) vs X**
- **V_{oc} (V) vs X**

Fig. 9
CdS (Buffer Layer)

- **Eta (%) vs X**
- **FF (%) vs X**
- **J_{sc} (mA/cm^2) vs X**
- **V_{oc} (V) vs X**

**Fig. 10**
**CH$_3$NH$_3$SnI$_3$ (Absorber Layer)**

- **$V_{oc}$ (V) vs X**
- **$J_{sc}$ (mA/cm$^2$) vs X**
- **FF (%) vs X**
- **Efficiency (%) vs X**

Fig. 11
Fig. 12
Performance of solar cell

- $\eta$ (%) vs $T$
- FF (%) vs $T$
- $J_{sc}$ (mA/cm$^2$) vs $T$
- $V_{oc}$ (V) vs $T$

Fig. 13
### Table 1

| Material Parameters | ZnO (ETM) | CdS (Buffer) | CH$_3$NH$_2$SnI$_3$ (Absorber) | GaAs (HTM) |
|---------------------|-----------|--------------|-------------------------------|-------------|
| Thickness (µm)      | 0.01 (variable) | 0.001 (variable) | 0.2 (variable) | 1.00 (variable) |
| Energy band-gap (eV)| 3.37      | 2.44         | 1.35                         | 1.42        |
| Electron Affinity   | 4.35      | 4.40         | 4.170                        | 4.07        |
| Dielectric Permittivity | 10.0    | 10.00        | 6.50                         | 12.9        |
| CB DOS              | 2.22E18   | 2.2E18       | 1.0E18                       | 2.2E18      |
| VB DOS              | 1.78E19   | 1.8E19       | 1.0E19                       | 1.8E19      |
| Electron/hole thermal velocity | 1E7 | 1E7 | 1E7 | 1E7 |
| Electron Mobility   | 100       | 100          | 10.0                         | 8500        |
| Hole Mobility       | 25        | 25           | 10.0                         | 400         |
| N$_d$               | 1E20      | 1E18         | 0                            | 0           |
| N$_a$               | 0         | 0            | 3.20E15                      | 1E11        |

### Table 2

| Material Parameters | CdS/ZnO Layer | CdS/CH$_3$NH$_2$SnI$_3$ Layer | CH$_3$NH$_2$SnI$_3$/GaAs Layer |
|---------------------|---------------|--------------------------------|--------------------------------|
| Defect type         | Neutral       | Neutral                        | Neutral                        |
| Capture cross section for Electrons and holes (/cm$^2$) | 1.0×10$^{-15}$ | 1.0×10$^{-15}$ | 1.0×10$^{-15}$ |
| Energy distribution | Single        | Single                         | Single                         |
| E- level w.r.t E$_v$ (above E$_v$,eV) | 0.6 | 0.6 | 0.6 |
| Total density N$_d$/cm$^3$ | 1.0×10$^{19}$ | 1.0×10$^{16}$ | 1.0×10$^{13}$ |
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