

Effect of Thickness of Absorber Layer on the Enhancement of Efficiency, and Performance of $\text{CH}_3\text{NH}_3\text{SnI}_3$ based Perovskite Solar Cell using SCAPS-1D

Km. Karishma¹, Abhishek Kumar Gupta^{2,*}, Omhari Dubey³, Sarvesh Kumar Gupta⁴

Abstract

The present research article deals with the improvement of efficiency, and performance of tin based perovskite solar cells (PSCs) using SCAPS-1D software. SCAPS-1D has been used for investigating the absorber layer of the inverted p-i-n arrangement of tin based perovskite solar cells. The inverted p-i-n solar cell arrangement are Glass/ITO/NiO/ $\text{CH}_3\text{NH}_3\text{SnI}_3$ /PCBM/AL where ITO, NiO, $\text{CH}_3\text{NH}_3\text{SnI}_3$, PCBM and Al are transparent conducting oxide, hole transporting layer (HTL), absorber layer and electron transporting layer (ETL) and back contact respectively. The approach to enhance the device efficiency is revealed in terms of structural and absorber layer effect. The thickness and defect density of the absorber layer, along with the acceptor density of the hole transporting layer, were simulated, leading to rise in solar cell performance. The power conversion efficiency of PSCs has been found to increase up to a sensible level as per simulation result obtained using SCAPS-1D software.

Keywords: Absorber layer, Inverted perovskite solar cells, NiO, PCBM, Defect density, acceptor density

*Author for Correspondence

Abhishek Kumar Gupta

^{1,3}Student, Nanoionics and Energy Storage Laboratory (NanoESL), Department of Physics and Material Science, Madan Mohan Malaviya University of Technology, Gorakhpur, Uttar Pradesh, India

²Assistant Professor, Nanoionics and Energy Storage Laboratory (NanoESL), Department of Physics and Material Science, Madan Mohan Malaviya University of Technology, Gorakhpur, Uttar Pradesh, India

⁴Research Scholar, Nanoionics and Energy Storage Laboratory (NanoESL), Department of Physics and Material Science, Madan Mohan Malaviya University of Technology, Gorakhpur, Uttar Pradesh, India

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INTRODUCTION

The energy demand is increasing with development in the world economy. According to cleaned, abundant, renewable energy the fossil fuels cannot fulfil the energy consumption. The solar cells are the best renewable energy sources. It attracted enormous attention due to limitless quality of solar energy and eco-friendly [1]. Third generations PSCs has attracted scientists because it is very efficient, low cost and excellent power conversion efficiency [2]. The band gap of p-type semiconductor NiO is wide and as hole transporting layer it has very good potential for solar energy conversion. Its optical transparency is excellent and chemical stability is also high [3]. Inverted p-i-n structure devices are easy to design. It has good stability, hysteresis effects negligible, good performance and applicable potential for flexible perovskite solar cell [4]. Whereas, the hysteresis effects are a major problem in progress of planar heterojunction perovskite solar cells [5]. Recently, with easy processing techniques and low cost the

lead free perovskite solar cell has created a great deal of attention in comparison to silicon based solar cells. In comparison to lead halide perovskite, lead free $\text{CH}_3\text{NH}_3\text{SnI}_3$ can cover extensive range of visible spectrum according to experimental and theoretical studies [6]. The planar hetero-junction structure is well suited to tin-based perovskite solar cells [1].

The inverted p-i-n solar cell Glass/ITO/NiO/ $\text{CH}_3\text{NH}_3\text{SnI}_3$ /PCBM/AL was examined using SCAPS-1D in this study. PSC output was examined when the thickness and defect density of the absorber layer, the acceptor density of the hole transporting layer, and the defect density of the interface were varied. The main objective of this simulation is to increase the lead-free perovskite solar cell's efficiency.

FRAMEWORK OF PSCS AND NUMERICAL ANALYSIS WITH SCAPS-1D

The inverted p-i-n solar cell structure is Glass/ITO/NiO/ $\text{CH}_3\text{NH}_3\text{SnI}_3$ /PCBM/AL where ITO is transparent conducting oxide, NiO is an inorganic p-type material which is used as HTL because of their greater stability, $\text{CH}_3\text{NH}_3\text{SnI}_3$ is perovskite material which is used as absorber layer, PCBM is considered as an ETL. Al is back contact material with the work function of 4.26 eV as shown in Figure 1 [5]. This simulation was done by using the SCAPS-1D software. The department of electronics and information technology of Gent University in Belgium developed the SCAPS-1D software.

SCAPS-1D (solar cell capacitance simulator) is comprised of three formulas. First is Poisson's equation, second continuity equation, and third transport equation [7, 8]. The simulation has been optimized at standard spectrum AM1.5G, working temperature 300 K by taking series resistance $1\ \Omega$ and shunt resistance $1 \times 10^6\ \Omega$ [9].

RESULT AND DISCUSSION

The inverted p-i-n solar cell structure Glass/ITO/NiO/ $\text{CH}_3\text{NH}_3\text{SnI}_3$ /PCBM/AL where ITO, NiO, $\text{CH}_3\text{NH}_3\text{SnI}_3$, PCBM and Al are transparent conducting oxide, HTL, absorber layer, ETL and back contact respectively. The simulation has been done by using parameters from Table 1.

Effect of thickness of absorber layer

The performance of solar cell is highly affected by the variation of thickness of the absorber layer. The absorber layer thickness ranged from 0 to $2.2\ \mu\text{m}$. Since thick absorber layer absorbed more photons, therefore more number of electron-hole pairs produced, and then parameters J_{SC} , V_{OC} and PCE increased with increasing absorber layer thickness and FF decreased.

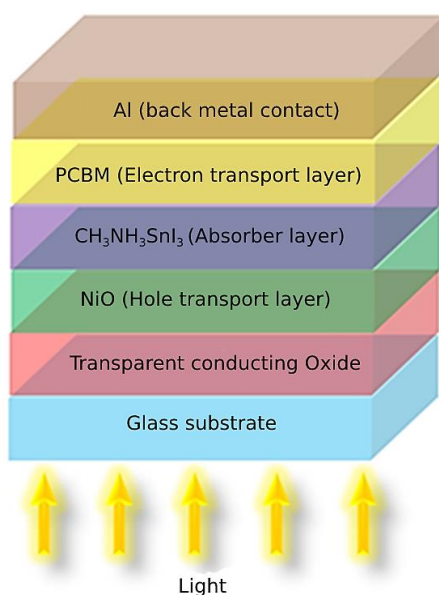


Figure 1. Device structure of PSCs.

Table 1. Lists of parameters used in simulation process [2].

Parameters	NiO	CH ₃ NH ₃ SnI ₃	PCBM
Thickness (μm)	0.03	2.0	0.085
Band gap E _g (eV)	3.8	1.3	2.0
Electron affinity χ (eV)	1.46	4.17	4.2
Dielectric affinity ε (relative)	11.7	10.00	3.900
CB effective density of states N _e (cm ⁻³)	2.500E+20	1.000E+19	2.500E+21
VB effective density of states N _v (cm ⁻³)	2.500E+20	1.000E+18	2.500E+21
Electron thermal velocity v _e (cm/s)	1.00E+7	1.00E+7	1.00E+7
Hole thermal velocity v _h (cm/s)	1.00E+7	1.00E+7	1.00E+7
Electron mobility μ _e (cm ² /V.s.)	2.8	1.6	0.20
Hole mobility μ _h (cm ² /V. s.)	2.8	1.6	0.20
Donor density N _D (cm ⁻³)	0.000E+0	3.000E+17	2.930E+16
Acceptor density N _A (cm ⁻³)	3.000E+21	3.000E+17	0.000E+0
Defect N _t (cm ⁻³)	1.000E+15	1.000E+10	1.000E+15

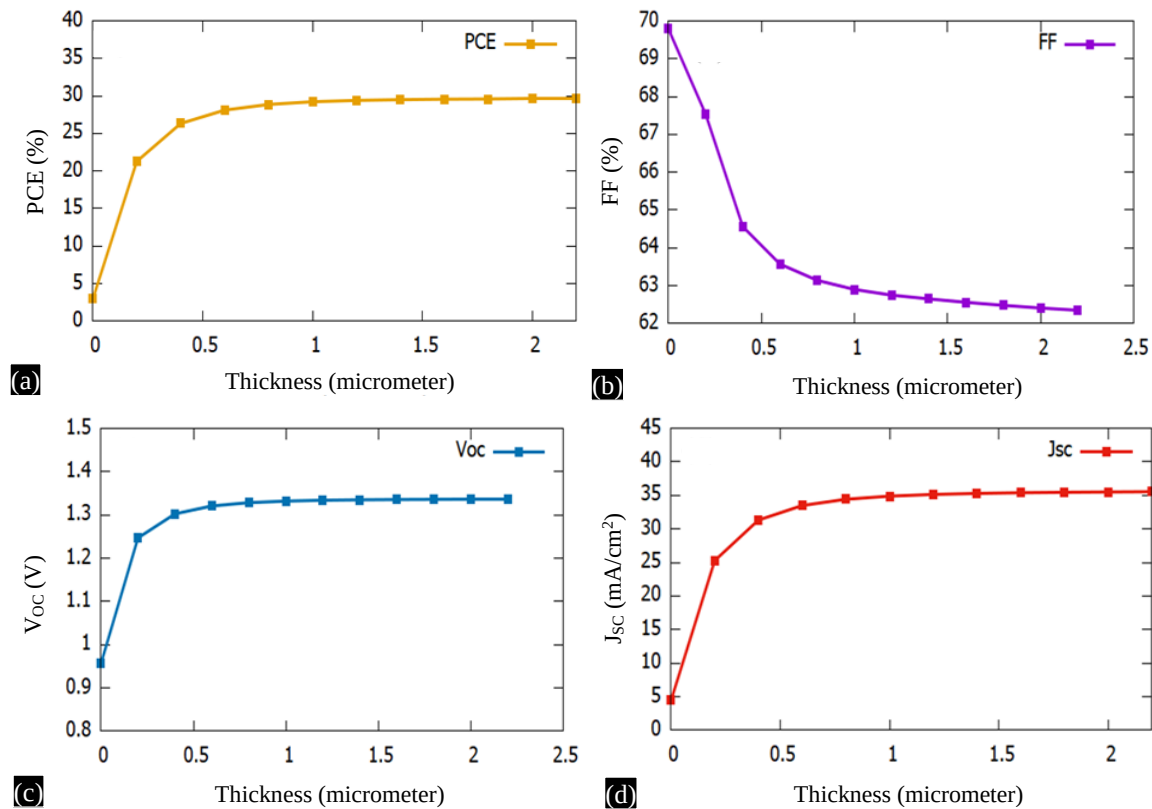


Figure 2. Effect of thickness of absorber layer on J_{SC}, V_{OC}, PCE and FF.

Charge carriers get divided due to electric fields and built-in-potential. From Figure 2(a-d), it was observed that J_{SC}, V_{OC}, PCE increase at a certain value and further constant because probability of recombination of charge carriers increased in thicker layer to movement longer distance for diffusion [10].

Effect of defect density of absorber layer.

The absorber layer defect density has a significant impact on solar cell performance. The absorber layer's defect density has been measured to be between 10⁹ and 10¹⁶ cm⁻³. With increasing defect density, it was observed that V_{OC}, J_{SC}, FF, and PCE all decreased.

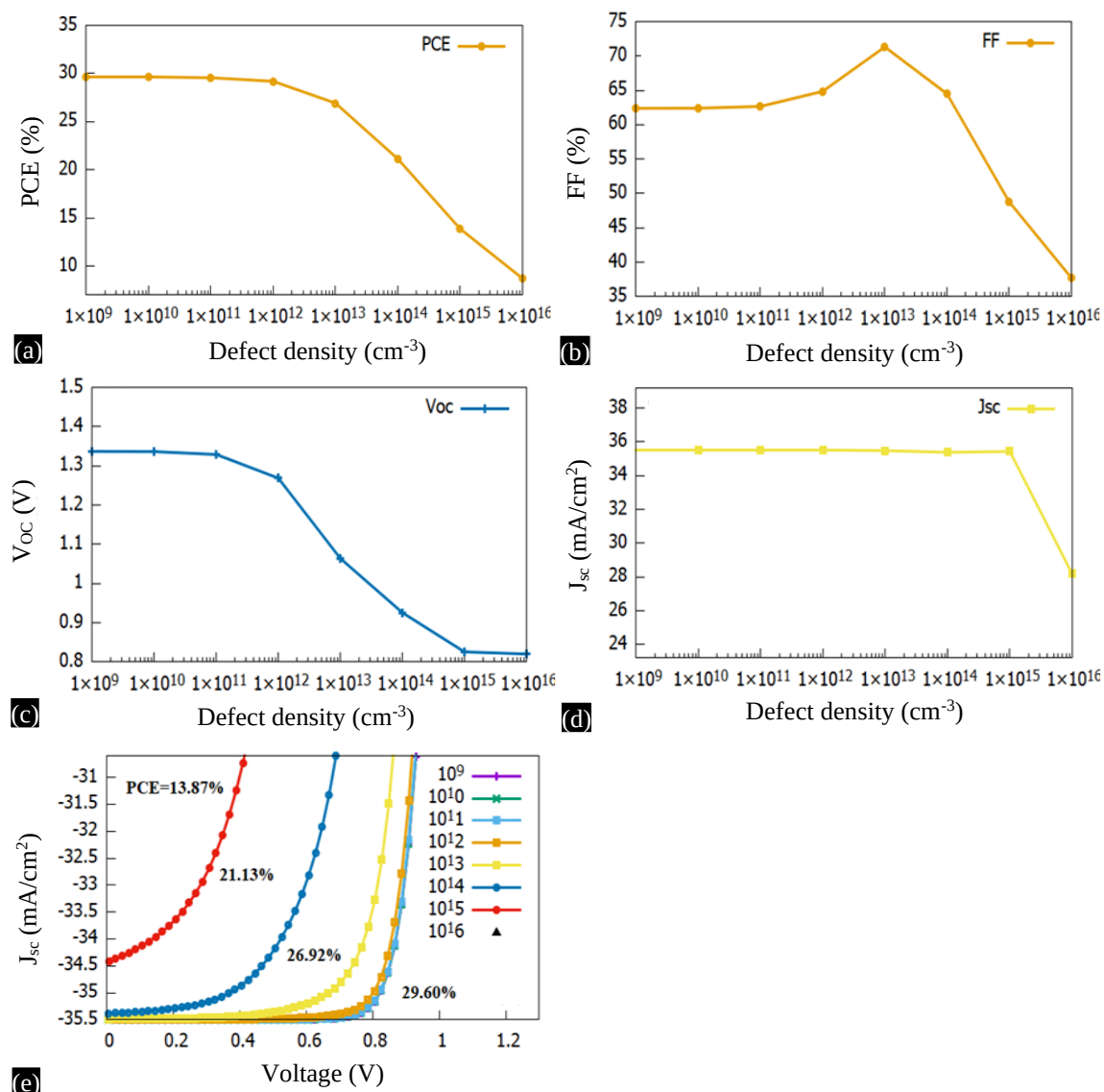


Figure 3. (a-e) Effect of defect density of absorber layer on J_{sc} , V_{oc} , PCE, FF and J-V curve.

As the density of defects increases, the lifetime of minority carriers decreases. As lifetime decreases, the diffusion length of electrons and holes reduce, causing recombination loss in the absorber layer to increase [11] as shown in Figure 3. At a defect density of 1010 cm⁻³, the parameters PCE (29.60%), FF (62.41%), V_{oc} (1.3361 V), and J_{sc} (35.495430 mA/cm²) were found, indicating that the solar cell performed efficiently.

Effect of acceptor density of NiO layer

Acceptor density of hole transporting layer was increased from 3×10¹⁶ to 3×10²¹ cm⁻³. The Figure 5 depicts that the PCE has been increasing with increasing N_A . The Figure 4 depicts that the PCE has been increasing with increasing acceptor density, because conductivity of NiO layer increased with high acceptor density. The PCE has been found 35.15% at acceptor density 3×10²¹ cm⁻³ [12].

Effect of interface defect density

Effect of defect density at NiO/CH₃NH₃SnI₃

The performance of photovoltaic devices is heavily influenced by interface defects. The defect density of NiO/CH₃NH₃SnI₃ interface is ranging from 10⁹ to 10¹⁶ cm⁻³ as shown in Figure 5 V_{oc} and PCE is decreased, FF is first increased then after decrease due to increased recombination of charge carriers

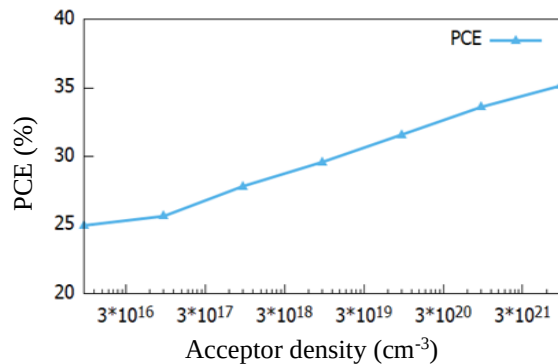


Figure 4. Effect of acceptor density of HTM layer on PCE.

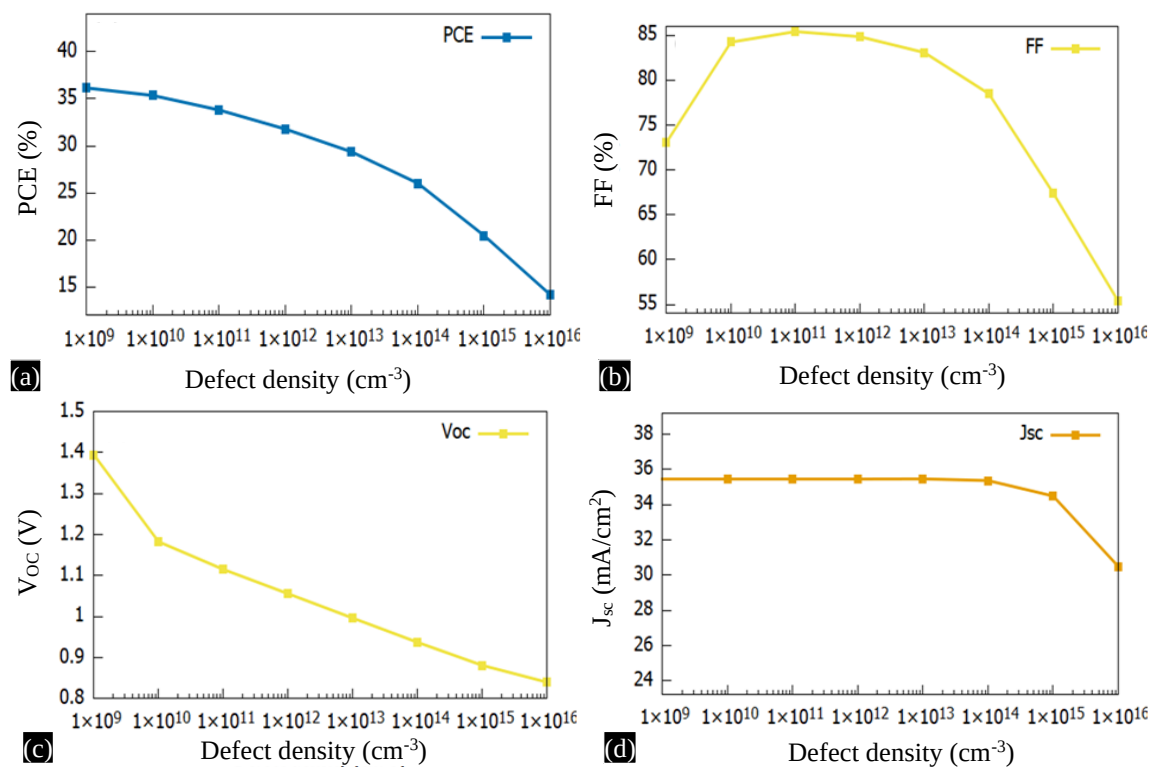


Figure 5. (a-d) Effect of defect density of interface defect layer NiO/CH₃NH₃SnI₃.

and shunt resistance changed. J_{SC} is slightly decreased due to series resistance increase [13]. The parameters value found PCE (35.34%), FF (84.25%), V_{OC} (1.1824 V) and J_{SC} (35.481189 mA/cm²) at 10¹⁰ cm⁻³ defect density interface defect layer NiO/CH₃NH₃SnI₃.

Effect of defect density at CH₃NH₃SnI₃/PCBM

The defect density of CH₃NH₃SnI₃/PCBM interface is ranging from 10⁹ to 10¹⁶ cm⁻³ as revealed in Figure 6 V_{OC} , J_{SC} , FF and PCE is decrease, because of increase in recombination of charge carriers [13]. The parameters value have been found as PCE (35.34%), FF (84.25%), V_{OC} (1.1824 V) and J_{SC} (35.481189 mA/cm²) at 10¹⁰ cm⁻³ interface defect density.

Optimized JV curve and Quantum efficiency

All simulated parameters, like absorber layer thickness, defect density, hole transporting layer acceptor density, and interface defect densities, have been combined and simulated for the J-V curve in this section.

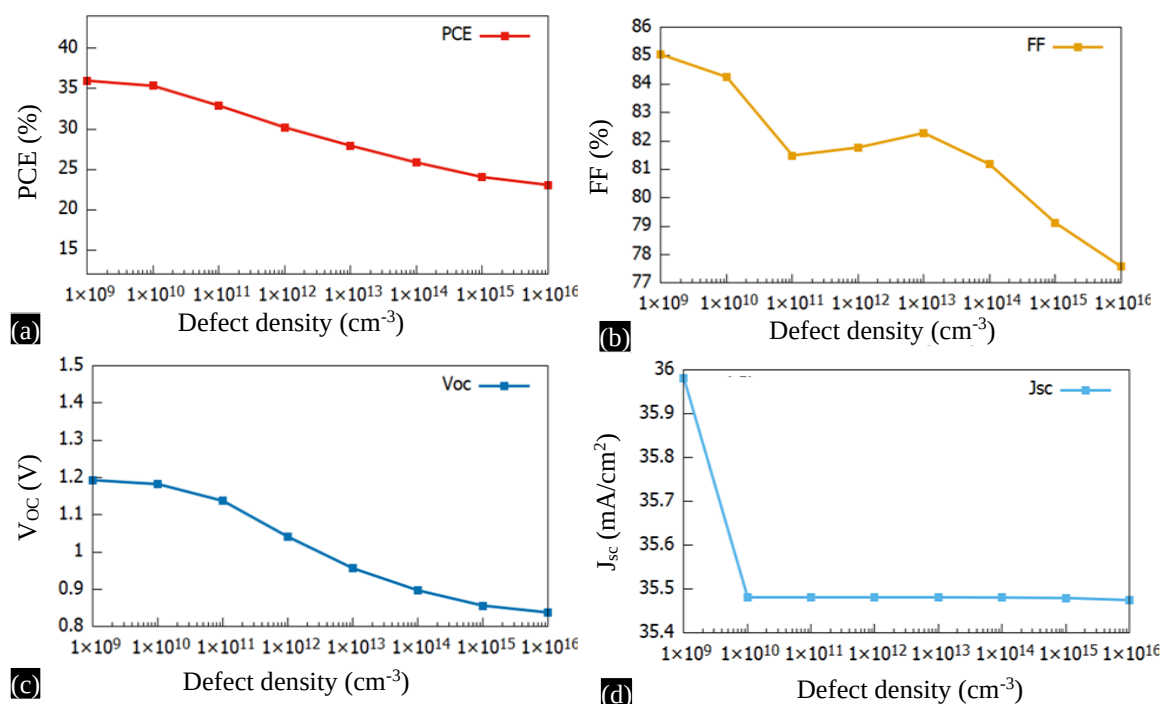


Figure 6. (a-d) Effect of defect density of interface defect layer CH₃NH₃SnI₃/PCBM.

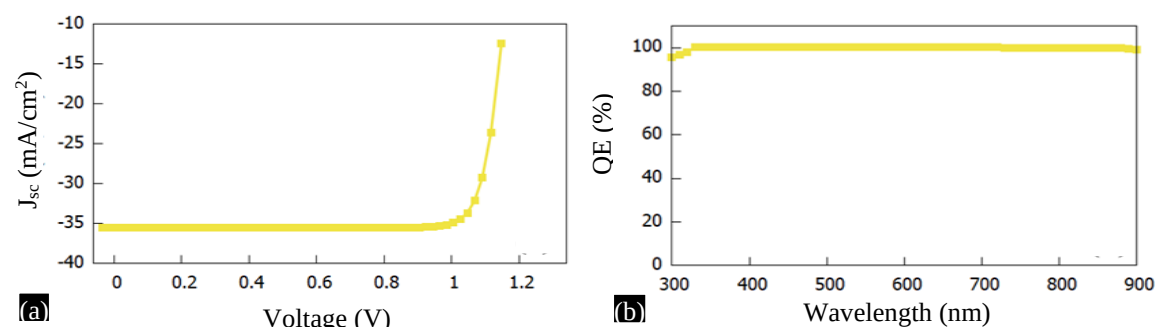


Figure 7. (a-b) Optimized JV curve and quantum efficiency with all simulated parameters of PSCs.

The J-V curve and quantum efficiency is shown in Figure 7(a and b). The parameters such as PCE (35.34%), FF (84.25%), Voc (1.1824 V) and Jsc (35.481189 mA/cm²) were observed.

CONCLUSION

In this simulation, the inverted p-i-n solar cell Glass/ITO/NiO/CH₃NH₃SnI₃/PCBM/Al has been investigated with the help of SCAPS-1D software. The impact of absorber layer thickness and defect density, HTM layer acceptor density, and interface defect were investigated. High performance perovskite solar cell found at thickness 2 μm, defect density 10¹⁰ cm⁻³ of absorber layer, acceptor density 3×10²¹ cm⁻³ of HTM layer and interface defect densities 10¹⁰ cm⁻³. PCE (35.34%), FF (84.25%), Voc (1.1824 V) and Jsc (35.481189 mA/cm²) is obtained.

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