

Modeling and Investigation of Highly Efficient Environment Friendly Perovskite Solar Cell with CuSbS_2 as Hole Transport Layer

Janendra Pratap, G.R. Mishra

Department of Physics & Electronics

Dr. Rammanohar Lohia Avadh University

Ayodhya, India

janendra1987@gmail.com, grmishra@gmail.com

Abstract— The presence of lead and its associated toxicity represents a hindrance to the broad commercial production of lead halide perovskites and their utilization in solar photovoltaic devices. Although lead halide perovskites have found extensive application in solar cell technology, questions have arisen regarding the hazardous nature and durability of lead (Pb) in photovoltaic systems. This research seeks to address these concerns by exploring alternative materials, such as tin-based perovskites, to pave the way for cleaner and more sustainable energy solutions. The scientific community has shown increased interest in tin-based perovskites due to their superior efficiency and stability compared to lead-based perovskite solar cell. This research introduces a planar heterojunction solar cell utilizing tin-based perovskites that are free of lead. The simulation task was conducted using SCAPS-1d software. Device parameters for a lead-free PSC (perovskite solar cell) using significant framework $\text{FTO}/\text{WS}_2/\text{CH}_3\text{NH}_3\text{SnI}_3$ (perovskite)/ CuSbS_2 included an examination of factors like perovskite layer thickness, the absorption of acceptors in the perovskite layer, defects density of perovskite layer, and the band gap of the perovskite layer. In this setup, WS_2 served as the ETL material, CuSbS_2 functioned as the HTL material, and the $\text{CH}_3\text{NH}_3\text{SnI}_3$ (Perovskite) was used as the absorber layer material. This configuration achieved an impressive PCE 32.5%, along with a J_{sc} 34.1 mA/cm^2 , V_{oc} 1.02V and FF 85.5%. These optimized results likelihood indicates the strong prospect for development of an eco-friendly and efficient model of PSC (perovskite solar cell).

Keywords- Lead-free perovskite Solar Cell, CuSbS_2 , WS_2 , SCAPS-1d

I. Introduction

During recent years the energy demand shoots up exponentially due to the technology and developments of the social infrastructure. The developed and developing countries both are depends upon the energy resources but the conventional energy resources are not enough to fulfill the demand and we have limited resources however, the photovoltaic technology based solar energy also participate to fulfill the global energy requirements moreover, the PV based solar energy is the eco-friendly and the eminent energy source to compete the traditional energy resources^{1,2}. In the PV-based solar cells the perovskite materials perform an ultimate character in photovoltaic technology. Many new perovskite materials have been found and optimized by the scientific community day by day for the better power conversion efficiency. The significant combination with organic substances and inorganic substances of PSC (perovskite solar cell) in modern era, it is next level solar cell device due to its PCE (power conversion efficiency). Many perovskite materials are using in current researches in which the lead (Pb) is the most promising material but the nature of lead is toxic and the stability of lead is very poor so that it is harmful for human and not suitable for environment as well as not fit for our eco-system. To overcome this issue the researchers and

scientists invented a lead-free perovskite $\text{CH}_3\text{NH}_3\text{SnI}_3$ material with certain optoelectronic standards and having band gap of 1.3 eV an appropriate range for absorber layer. Freshly, many scientists and researchers have successfully simulated/fabricated organic-inorganic material based PSC with good power conversion efficiency¹.

The perovskite basically illustrated with formula RMX_3 ² (where R stand for alkyl group M for metal and X for halogen). Perovskite materials having immersing features of excessive absorbing coefficient, high current mobility, low carrier recombination loss, extensive diffusion length and harmonious band gap with these properties making it a suitable for advance photovoltaic technology³. Typically, the framework of PSC (perovskite solar cell) comprises various key components, containing an ETL (electron transport layer), a HTL (hole transport layer), a perovskite layer, as well as a substrate composed of FTO (Fluorine-Doped Tin Oxide) and coated-glass⁴. In this simulation, FTO was taken due to its transparent nature, antireflection coating and its ohmic contact. Stability of PSC is key factor for commercialization purpose however, following factors are responsible for the degradation of the perovskite (a) Perovskite itself is a cause of the degradation, (b) surface indignity (c) Chemical taint⁵ (d) UV radiation also a major cause for the degradation of PSC.

In this research, we have chosen to incorporate n-type WS₂ (Tungsten disulfide) as the ETL material because of its remarkable optoelectronic characteristics⁶. WS₂ possesses a broad band-gap array spanning (1.3 - 2.2 eV), making it particularly suitable for our purposes. Its outstanding electron transport capability, attributed to its high electron mobility, is another compelling reason for its selection. Furthermore, we have the capability to modify the electronic attributes of WS₂ by applying external forces or introducing dopant atoms, allowing us to customize its structure to meet our particular needs. WS₂ used as ETL layer material instead of conventional TiO₂ it gives well response and results but TiO₂ had some limitations as well as some drawbacks like its degradation factor with time being under sustain UV- illumination and oxygen vacancy would turn in surface traps. The importance of the HTL is critical for attaining large PCE (power conversion efficiency) in PSC. The HTL's primary role is to uphold charge balance, inhibit charge recombination, and ultimately boost the overall performance of the PSC. Over the years, Spiro-OmeTAD has become the preferred material for HTL (hole transport layer). However, there are specific constraints associated with its utilization, including its elevated cost, limited availability due to its rarity, and its poor stability. In this simulation, we opt CuSbS₂ due to its plenty availability on across the globe, cost efficient and we matched band arrangements with our perovskite (CH₃NH₃SnI₃) material⁸. Simulation of any device provides a strong way to enhance perovskite solar cells efficiency by optimize the various photovoltaic parameters. SCAPS-1D distinguishes itself as an exceptionally reliable option for simulating solar cells because of its capacity to precisely forecast vital parameters, including J_{sc}, Voc, PCE, and FF in perovskite solar cells (PSCs)^{9,10}. As a result, this software was utilized for the exploration of an eco-friendly, without lead solar cell based on CH₃NH₃SnI₃. This simulation provided an opportunity for a comprehensive analysis of the operational behavior and functional characteristics of a perovskite solar cell (PSC) built with CH₃NH₃SnI₃.

II. Structure of Device and Numerical Simulation

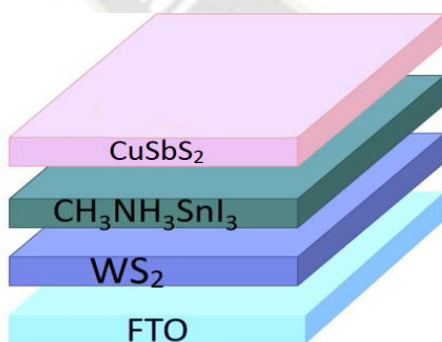


Figure 1. Lead-free CH₃NH₃SnI₃ based perovskite solar structure

In this investigation, mathematical simulations were performed on a planar heterojunction without lead tin based PSC using SCAPS 1d software, developed under the umbrella

of Gent-Zwignarde University, Belgium (Burgelman et. al., 2018). The simulated device structure constituted several layers like; FTO, ETL (buffer-layer), perovskite layer and HTL. Simulation process was conducted under standard AM1.5G spectrum illumination, with an effective intensity 1000W/m² and at 300K temperature.

The device diagrammatic representation is provided in (Fig. 1). In this depiction, the ETL is composed of n-type WS₂, the absorber layer is made of CH₃NH₃SnI₃, and the HTL is constructed from p-type CuSbS₂. FTO serves as the contact material, while an array of materials, including Pt, Ag, Cu, and Au, is utilized as the anode material.

To acquire the device parameters, such as energy band alignment, QE (quantum-efficiency) and J-V (current-density voltage) properties, the Poisson's continuity equation for electrons (holes) is applied. The resulting curves are then employed to determine the key parameters of the solar cell device.

Poisson's equation establishes the correlation between the electric-field intensity at p-n junction and space charges density⁵.

$$\frac{d}{dx} \left(-\epsilon(x) \frac{d\phi}{dx} \right) = [qp(x) - qn(x) + qN_D(x) - qN_A(x) + qp(x) - qn(x)] \quad (1)$$

Where, N_D denoted for donor concentration, N_A denoted for acceptor concentration, ρ denoted for the free hole density, n(x) represented the mobility of electron and p(x) stand for the hole mobility, ε denoted for constant of the dielectric medium. The continuity equations for holes(electrons) in steady-state can be articulated as follows;

$$\frac{\partial j_n}{\partial x} + G - U_n(n, p) = 0 \quad (2)$$

$$-\frac{\partial j_p}{\partial x} + G - U_p(n, p) = 0 \quad (3)$$

In the above equations, j_{n(p)} represent the current densities of electron (hole). U_{n(p)} is used to indicate the electron (hole) mobility, while G stands for rate of electron (hole) generation . The current density of electrons (holes) is showed as follows:

$$J_n = q \left[nu_n E + D_n \frac{dn}{dx} \right] \quad (4)$$

$$J_p = q \left[pu_p E - D_p \frac{dp}{dx} \right] \quad (5)$$

In the above equations D_{n(p)} is stand for diffusion coefficient of electron (hole); while q denoted the elementary charge.

The material parameters and their values have been sourced from a range of literature, research studies, and experimental findings, as summarized in Table 1. Typically, layer thickness is measured in nanometers (nm). The variables and their symbols include: E_g(band gap), χ (electron affinity), ε_r(proportional relative permittivity), N_v(state density of the valence band), N_A(acceptor-density), N_D(donor density), and N_r¹(defect-density). Additionally, the thermic velocities for electrons(holes) have been set at 10⁷ cms⁻¹.

III. Results and Discussion

The SCAPS-1d simulator used the tabulated parameters which are collected from various experimental and theoretical research papers to perform the simulation. The J-V characteristic and quantum efficiency of the PSC were generated from the data present in Table 1 and described in Fig. 2a and 2b. When the absorber (perovskite) layer is exposed into the sunlight, it generates electron-hole pairs. These pairs then migrate toward the ETL and HTL, where they are collected at anode and cathode, respectively. However, the electrons and holes are converted into voltage and we get the results of J_{sc} 34.11 mA cm⁻², V_{oc} 1.02 V, FF 85.55% and PCE 29.86%. The J_{sc} is one of the crucial parameter to characterize the PSC device parameters it depends on various elements such as efficiency, solar cell material properties, sunlight intensity and the formation of solar cell. Higher J_{sc} values means the solar cell can produce the more current, which is generally desirable for achieving the overall high efficiency from converting sunlight into electricity^{11,12}. The thicknesses of the absorber layer is primary determining factor in PSC since, it serve as a main method of absorbing solar radiation that has the highest cut-off wavelength. Consequently, the absorber layer's thickness has been carefully selected for this study to ensure optimal performance¹². The mobility values for both electrons and holes were obtained from recent research studies and employed in this investigation^{13,14}. The high value of J_{sc} was obtained because the charge carrier mobility is linearly proportional to the current density. The values of electron and hole mobility nevertheless, had been evaluated by Khattak et al. and Devi et al. to be quite small and identical. High mobility of charge carriers causes the diffusion length increase, which reduces the recombination of charge carrier¹⁴. The entirely visible spectrum's quantum efficiency curve is obtained in this investigation (Fig. 2b). It is possible to perform further studies to improve photovoltaic (PV) performance.

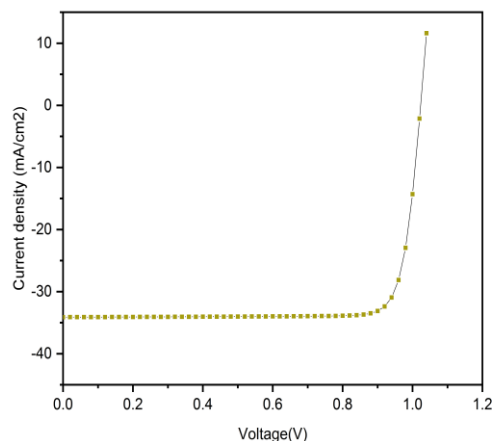


Figure 2a. J-V characteristic

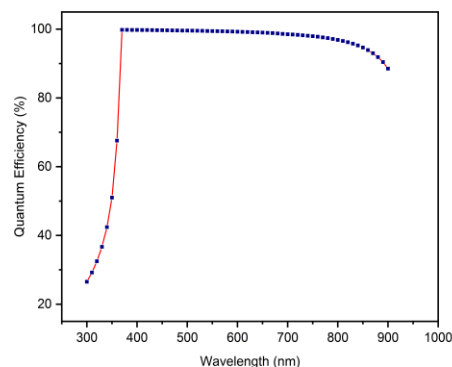


Figure 2b. PSC Quantum efficiency

Table 1. Optoelectronic simulation parameters

Parameters	FTO	WS ₂ (ETL)	CH ₃ NH ₃ SnI ₃ (absorber)	CuSbS ₂ (HTL)
Thickness (nm)	500	50	1000	50
E _g (eV)	3.4	1.8	1.3	1.58
χ (eV)	4.4	3.95	4.17	4.2
ε _r	9.1	13.6	10	14.6
N _c (cm ⁻³)	1.1x10 ¹⁹	2.2x10 ²¹	1.0x10 ¹⁸	2.0x10 ¹⁸
N _v (cm ⁻³)	1.1x10 ¹⁹	2.2x10 ¹⁶	1.0x10 ¹⁹	1.0x10 ¹⁹
μ _e (cm ² V ⁻¹ s ⁻¹)	20	100	1.6	49
μ _h (cm ² V ⁻¹ s ⁻¹)	10	100	1.6	49
N _D (cm ⁻³)	1.1x10 ¹⁹	1.0x10 ¹⁸	0	-

N_A (cm ⁻³)	-	-	1.0×10^{17} (variable)	1.38×10^{18}
N_t (cm ⁻³)	1.0×10^{14}	1.0×10^{15}	1.0×10^{14}	1.0×10^{14}

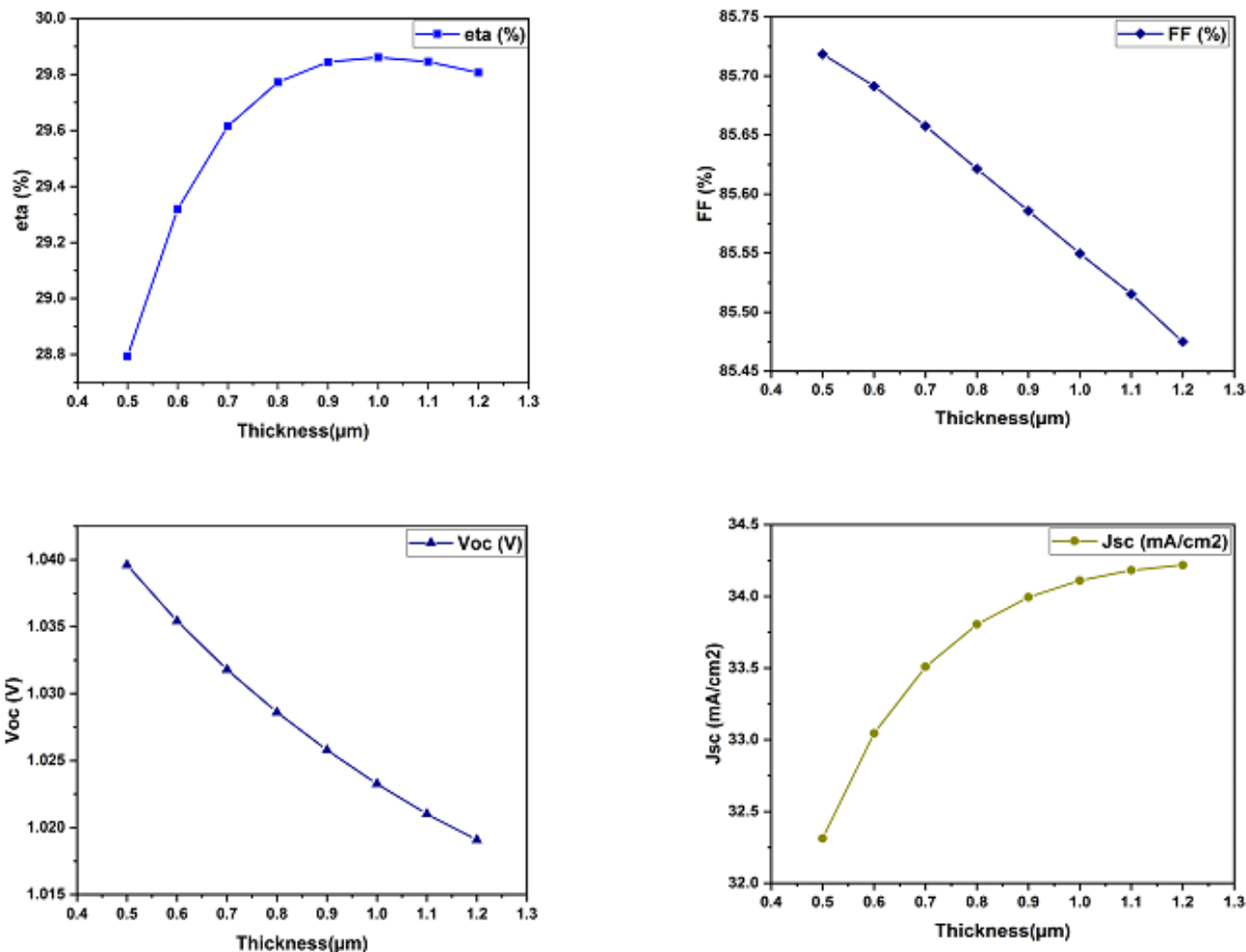


Figure 3 Effect of variation in perovskite layer thickness on various photovoltaic parameters

A. Absorber layer thickness

Numerous research studies have demonstrated that the absorber (perovskite) layer's thickness has considerable strike on critical PV (photovoltaic) parameters, including *PCE* (photo conversion efficiency), *FF* (fill factor), *Jsc* (short-circuit current density) and *Voc* (open-circuit voltage)^{15,16}. In this simulation, the perovskite layer thickness was diversified within the range of 400nm to 1200nm, while other parameters keeping fixed according to Table 1. The simulation results changed in response to the variation in perovskite layer thickness. The values of *Jsc* exhibited a rapid increase up to 1000 nm, after which they showed a gradual change with thickness variation. The highest *Jsc* value (~34.21 mA cm⁻²)

was achieved with a thickness of 1200 nm¹², primarily because of the significant recombination of free charge carriers in the thicker perovskite layer. Initially, there was an upward trend in power conversion efficiency (PCE), reaching its peak value (~29.86%) at 1000 nm. However, as the perovskite layer thickness continued to increase, PCE started to decrease. This phenomenon is attributed to the diffusion length of the charge carriers being greater than the thickness of the absorber layer. Consequently, the majority charge carriers reached at the electrode, resulting in an enhanced PCE (Fig. 3). Nevertheless, in thicker absorber layers, recombination became more pronounced, leading to a decline in PCE as the absorber thickness increased further¹⁷.

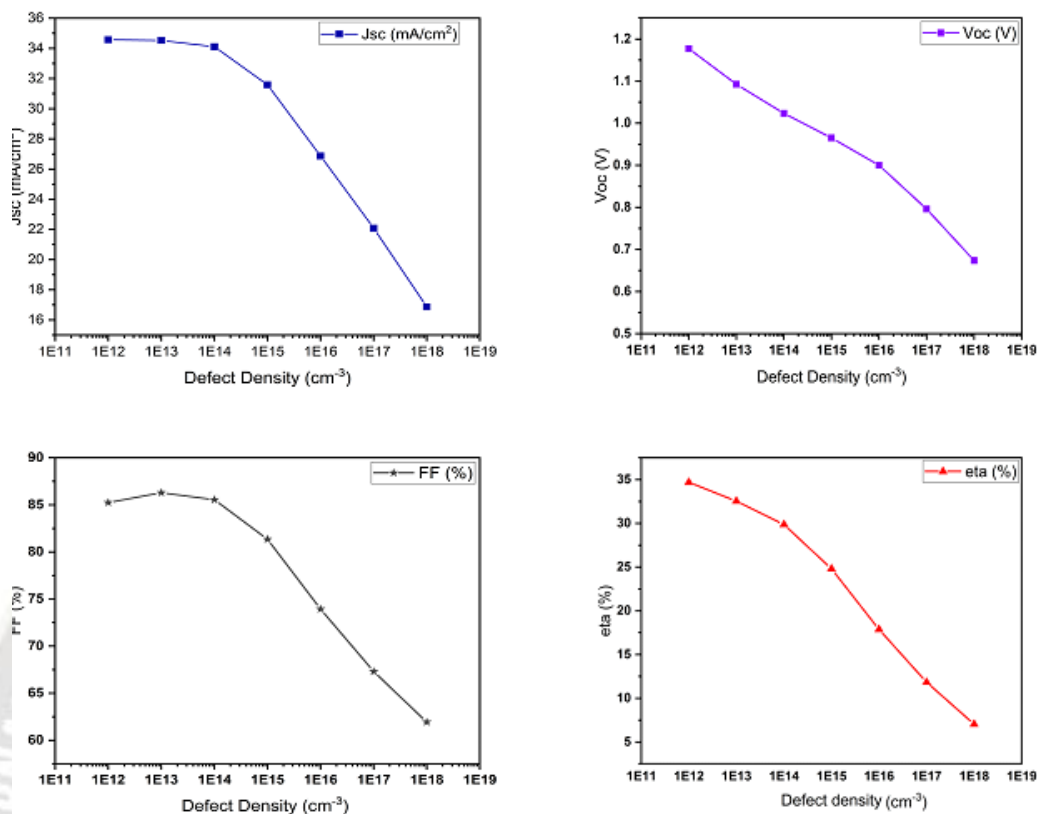


Figure 5 Impact of varying defect density on different photovoltaic parameters

B. Perovskite layer acceptor carrier concentration (N_A)

In addition to the thickness of the perovskite layer, another critical factor affecting the performance of photovoltaic devices is the density of acceptors for holes within the perovskite layer. When any device is exposed to air, the oxides in the perovskite layer undergo a self-doping phenomenon, changing from Sn²⁺ to Sn⁴⁺. Unfortunately, this self-doping process diminishes the device's performance while creating a p-type semiconductor^{18,19}. The transformation from Sn²⁺ to Sn⁴⁺ can be mitigated by incorporating SnO₂²⁰. Dark carrier densities, ranging from 10¹⁴cm⁻³ to 10¹⁷cm⁻³, were calculated by Feng et al., and according to Takashi et al., the hole concentration in the perovskite absorber layer can be varied till 10¹⁹cm⁻³. In this research, the acceptor density within the perovskite layer was systematically altered, spanning from 10¹⁴cm⁻³ to 10¹⁹cm⁻³, to assess the impact of acceptor doping concentration on photovoltaic device parameters. (Fig.4a & 4b) Illustrate the resulting variations in PCE and J-V characteristics concerning the acceptor density within the perovskite absorber layer²¹. Relatively minor changes in photovoltaic parameters were observed within the acceptor concentration range of up to 10¹⁸cm⁻³, indicating that the rate of generating photo-induced charge carriers remains relatively stable, regardless of variations in acceptor densities when exposed to the same number of incident photons^{22,23}. With an increase in acceptor doping concentration, there is a corresponding decrease in Fermi energy level of the holes, leading to an increase in Voc, as shown in (Fig. 4a).

Additionally, it's important to note that the built-in potential increases with higher acceptor doping concentrations. This may be attributed to the concept of charge dissociation. Initially, the Jsc showed a gradual decrease up to an acceptor concentration of 10¹⁸cm⁻³. However, beyond this point, a sharp decline in Jsc became evident. This decrease in Jsc may be attributed to an increase in the rate of charge carrier recombination within the perovskite layer. In contrast, power conversion efficiency (PCE) demonstrated a significant decrease as the acceptor density exceeded 10¹⁸cm⁻³, as depicted in (Fig. 4b).

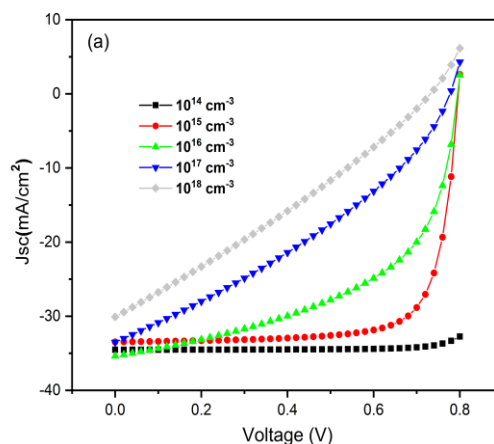


Figure 4(a). J-V curve for various acceptor density

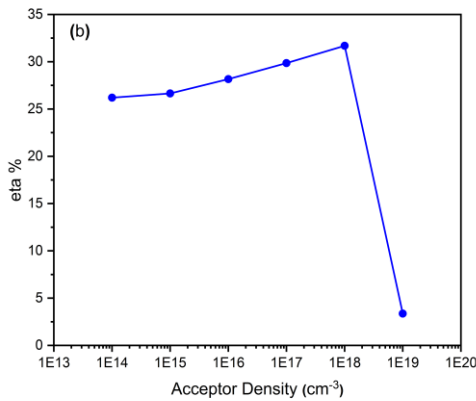


Figure 4(b). acceptor density versus efficiency

C. Impact of defect density (N_t) on the perovskite layer

Defects are naturally present in PSC, and the aim of this study was to investigate the impact of defect density within the perovskite layer. The perovskite layer consist various point defects, including Frenkel defects, lattice vacancies, interstitial defects and Schottky defects. A self-doping process introduces impurity defects into the perovskite layer, leading to the

creation of a p-type semiconductor^{24,25,26}. These defects cause variations in the energy band gap, enabling them to trap charge carriers (electrons and holes) without radiative emission. Remarkably, the use of a tin-reduced precursor solution has been observed to increase diffusion span of the charge carriers in tin-based perovskite layers to approximately 3 μm. Consequently, there is a clear correlation between defect density and diffusion span of the charge carriers. In this research, the defect-density within the perovskite layer was methodically adjusted, ranging from 10¹⁷cm⁻³ to 10¹⁸cm⁻³, to probe its consequences on the PV characteristics of PSC. The findings indicated that decreasing defect density led to an enhancement in device performance. Conversely, as defect density increased, there was a substantial improvement in cell performance, achieving notable values for Voc at 1.02 V, Jsc at 34.1 mA/cm², FF at 85.5% and PCE at 29.9% . Further reductions in defect density, from 10¹⁴cm⁻³ to 10¹³cm⁻³, resulted in slight variations in Jsc at 34.5 mA·cm⁻² and FF at 86.3%, but significant changes were observed in Voc at 1.09 V and PCE at 32.5%. This exceptionally high mobility led to a significant diffusion length, providing to the impressive PCE of 32.5%. This remarkable achievement can be attributed to the combination of a low recombination-rate and an extensive diffusion span (length). Therefore, the results obtained in this study surpass previously published results and demonstrate superior performance^{27,28,29}.

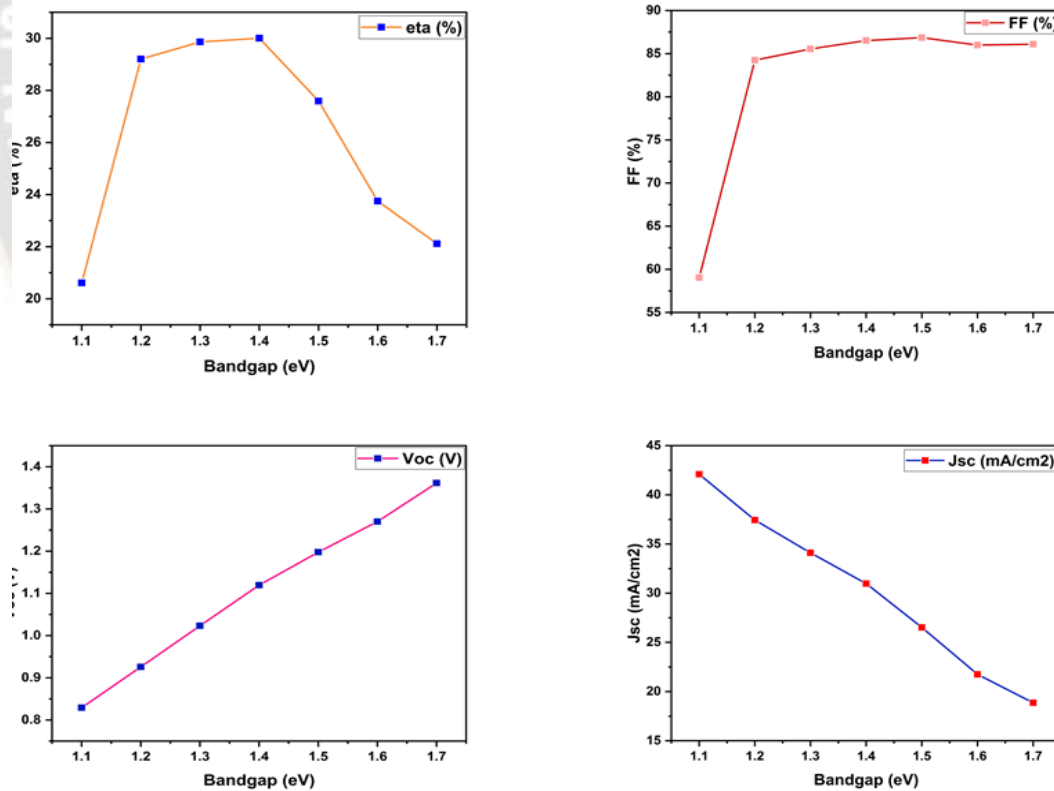


Figure 6 (a). Effect of absorber bandgab variation on solar cell parameters

D. Impact of band gap on the perovskite layer

Solar cell's efficiency is significantly affected by the band gap of its perovskite layer, as this band gap determines the spectrum of light wavelengths that the solar cell can efficiently capture^{30,31}. Wider band gaps are well-suited for capturing high-energy photons, while narrower band gaps are more efficient for lower-energy photons^{32,33}. The choice of absorber material and its specific band gap significantly impacts on the solar cell's efficiency and overall performance whereas, affecting key factors such as Voc, Jsc, and PCE.

Hence, understanding and optimizing the perovskite layer's band gap is fundamental in the design and enhancement of efficient solar cells. The photovoltaic parameters exhibited variations as the perovskite layer's band gap spanned from 1.1 eV to 1.7 eV, as depicted in (Fig. 6a). As the perovskite layer's band gap increased, both the FF and Voc also increased. Conversely, the Jsc and PCE decreased with an increase in the perovskite layer's band gap. (Fig. 6a) Illustrates that the PCE reaches its peak at 1.3 eV; however, any further growth in the band gap results in reduce in PCE. (Fig. 6b) illustrates, the QE (quantum efficiency) of the absorber layer at various band gap values. It's evident that QE is highest when the band gap is lower, particularly at 1.2 eV. As the absorber band gap values increase, the QE decreases. This reduction in QE has direct impact on both PCE and Jsc in the PSC (perovskite solar cell) device, leading to a decline in these performance parameters.

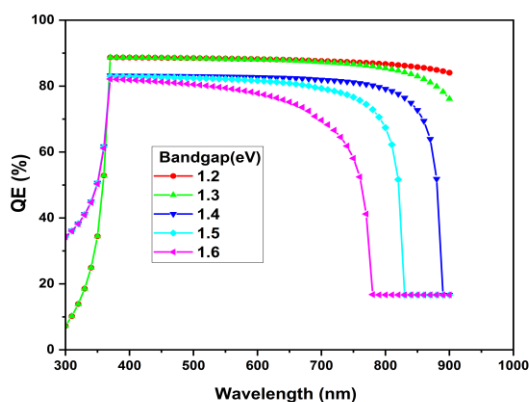


Figure 6 (b).QE versus wavelength

IV. Conclusion

In this current investigation, a without-lead heterojunction PSC structure, comprising FTO/WS₂/CH₃NH₃SnI₃/CuSbS₂/anode, was thoroughly examined both graphically and systematically. The study revealed that lead-free PSC have the potential to serve as efficient light-harvesters. To optimize the efficiency of these cells, several parameters were investigated, including perovskite layer thickness, band gap, acceptor density, and defect density.

The highest PCE (power conversion efficiency) achieved 29.91%, particularly higher than the results of previous studies, and it occurred with perovskite layer thickness of 1000nm. Additionally, it was observed that PCE increased

with defect density increases up to a certain point (*i.e.*, up to N_t value of 10^{14} cm⁻³). Beyond this threshold, a higher defect density led to an increased rate of carrier charge recombination, adversely affecting the overall cell performance. The results obtained from this simulation work point to the potential for developing environmentally friendly, non-toxic and highly efficient perovskite devices for future generations. This research contributes to the advancement of sustainable and high-performance solar cell technology.

Acknowledgments

The authors extend their appreciation to Dr. Marc Burgelman from the University of Gent, Belgium, for generously sharing the SCAPS-1d simulation software.

References

- [1] Patel, P.K. Device simulation of highly efficient eco-friendly CH₃NH₃SnI₃ perovskite solar cell. *Sci Rep* 11, 3082 (2021).
- [2] K. Domanski, E.A. Alharbi, A. Hagfeldt, M. Grätzel, W. Tress, Systematic investigation of the impact of operation conditions on the degradation behaviour of perovskite solar cells. *Nat. Energy* 3, 61–67 (2018).
- [3] [Song Li;Yong-LiCao;Wen-HuaLi;Zhi-Shan Bo; (2021). A brief review of hole transporting materials commonly used in perovskite solar cells . *Rare Metals*, (), -. doi:10.1007/s12598-020-01691-z]
- [4] [M.F. Mohamad Noh, C.H. Teh, R. Daik, E.L. Lim, C.C. Yap,M.A. Ibrahim, N. Ahmad Ludin, A.R. Bin MohdYusoff, J. Jang, M. Teridi, The architecture of the electron transport layer for a perovskite solar cell. *J. Mater. Chem. C* 6, 682–712 (2018). <https://doi.org/10.1039/c7tc04649a>]
- [5] Azri, Faiza, AfakMeftah, NouredineSengouga, and AmjadMeftah. "Electron and hole transport layers optimization by numerical simulation of a perovskite solar cell." *Solar energy* 181 (2019): 372-378
- [6] Kumar, Anjan, and Sangeeta Singh. "Numerical modeling of planar lead free perovskite solar cell using tungsten disulfide (WS₂) as an electron transport layer and Cu₂O as a hole transport layer." *Modern Physics Letters B* 34, no. 24 (2020): 2050258.
- [7] Sharma, Divya, Rajesh Mehra, and Balwinder Raj. "Optimization of tin based perovskite solar cell employing CuSbS₂ as HTL: A numerical simulation approach." *Optical Materials* 134 (2022): 113060.
- [8] Yang, Bo, Liang Wang, Jun Han, Ying Zhou, Huaibing Song, Shiyong Chen, JieZhong, Lu Lv, DongmeiNiu, and Jiang Tang. "CuSbS₂ as a promising earth-abundant photovoltaic absorber material: a combined theoretical and experimental study." *Chemistry of Materials* 26, no. 10 (2014): 3135-3143.)
- [9] Wang, Yan, Zhonggao Xia, Jun Liang, Xinwei Wang, Yiming Liu, Chuan Liu, Shengdong Zhang, and Hang Zhou. "Towards printed perovskite solar cells with cuprous oxide hole transporting layers: a theoretical

- design." *Semiconductor Science and Technology* 30, no. 5 (2015): 054004.
- [10] Du, Hui-Jing, Wei-Chao Wang, and Jian-Zhuo Zhu. "Device simulation of lead-free $\text{CH}_3\text{NH}_3\text{SnI}_3$ perovskite solar cells with high efficiency." *Chinese Physics B* 25, no. 10 (2016): 108802.
- [11] Stranks, Samuel D., Giles E. Eperon, Giulia Grancini, Christopher Menelaou, Marcelo JP Alcocer, Tomas Leijtens, Laura M. Herz, Annamaria Petrozza, and Henry J. Snaith. "Electron-hole diffusion lengths exceeding 1 micrometer in an organometal trihalide perovskite absorber." *Science* 342, no. 6156 (2013): 341-344.
- [12] Lin, Lingyan, Linqin Jiang, Ping Li, Baodian Fan, and Yu Qiu. "A modeled perovskite solar cell structure with a Cu_2O hole-transporting layer enabling over 20% efficiency by low-cost low-temperature processing." *Journal of Physics and Chemistry of Solids* 124 (2019): 205-211.
- [13] Lazemi, Masoud, Saeid Asgharizadeh, and Stefano Bellucci. "A computational approach to interface engineering of lead-free $\text{CH}_3\text{NH}_3\text{SnI}_3$ highly-efficient perovskite solar cells." *Physical Chemistry Chemical Physics* 20, no. 40 (2018): 25683-25692.
- [14] Hao, Feng, Constantinos C. Stoumpos, Duyen Hanh Cao, Robert PH Chang, and Mercouri G. Kanatzidis. "Lead-free solid-state organic-inorganic halide perovskite solar cells." *Nature photonics* 8, no. 6 (2014): 489-494.
- [15] Son, Dae-Yong, Jeong-Hyeok Im, Hui-Seon Kim, and Nam-Gyu Park. "11% efficient perovskite solar cell based on ZnO nanorods: an effective charge collection system." *The Journal of Physical Chemistry C* 118, no. 30 (2014): 16567-16573.
- [16] Ma, Lin, Feng Hao, Constantinos C. Stoumpos, Brian T. Phelan, Michael R. Wasielewski, and Mercouri G. Kanatzidis. "Carrier diffusion lengths of over 500 nm in lead-free perovskite $\text{CH}_3\text{NH}_3\text{SnI}_3$ films." *Journal of the American Chemical Society* 138, no. 44 (2016): 14750-14755.
- [17] Takahashi, Yukari, Hiroyuki Hasegawa, Yukihiko Takahashi, and Tamotsu Inabe. "Hall mobility in tin iodide perovskite $\text{CH}_3\text{NH}_3\text{SnI}_3$: Evidence for a doped semiconductor." *Journal of Solid State Chemistry* 205 (2013): 39-43.
- [18] Noel, Nakita K., Samuel D. Stranks, Antonio Abate, Christian Wehrenfennig, Simone Guarnera, Amir-Abbas Haghgheirad, Aditya Sadhanala et al. "Lead-free organic-inorganic tin halide perovskites for photovoltaic applications." *Energy & Environmental Science* 7, no. 9 (2014): 3061-3068.
- [19] Lee, Young Mi, Inhee Maeng, Jinwoo Park, Myungkwan Song, Jung-Ho Yun, Min-Cherl Jung, and Masakazu Nakamura. "Comprehensive understanding and controlling the defect structures: An effective approach for organic-inorganic hybrid perovskite-based solar-cell application." *Frontiers in Energy Research* 6 (2018): 128.
- [20] Lin, Renxing, Ke Xiao, Zhengyuan Qin, Qiaolei Han, Chunfeng Zhang, Mingyang Wei, Makhsud I. Saidaminov et al. "Monolithic all-perovskite tandem solar cells with 24.8% efficiency exploiting comproportionation to suppress Sn (ii) oxidation in precursor ink." *Nature Energy* 4, no. 10 (2019): 864-873.
- [21] Devi, Chandni, and Rajesh Mehra. "Device simulation of lead-free MASnI_3 solar cell with CuSbS_2 (copper antimony sulfide)." *Journal of materials science* 54 (2019): 5615-5624.
- [22] Lin, Renxing, Ke Xiao, Zhengyuan Qin, Qiaolei Han, Chunfeng Zhang, Mingyang Wei, Makhsud I. Saidaminov et al. "Monolithic all-perovskite tandem solar cells with 24.8% efficiency exploiting comproportionation to suppress Sn (ii) oxidation in precursor ink." *Nature Energy* 4, no. 10 (2019): 864-873.
- [23] Dai, Shuxi, Yanqiang Wu, Toshio Sakai, Zuliang Du, Hideki Sakai, and Masahiko Abe. "Preparation of highly crystalline TiO_2 nanostructures by acid-assisted hydrothermal treatment of hexagonal-structured nanocrystalline titania/cetyltrimethylammonium bromide nanoskeleton." *Nanoscale research letters* 5, no. 11 (2010): 1829-1835.
- [24] Peng, Huirong, Molang Cai, Jiyu Zhou, Yi Yang, Xihong Ding, Ye Tao, Gao Wu, Xuepeng Liu, Jia Hong Pan, and Songyuan Dai. "Structurally Reinforced All-Inorganic CsPbI_2Br Perovskite by Nonionic Polymer via Coordination and Hydrogen Bonds." *Solar RRL* 4, no. 9 (2020): 2000216.
- [25] Stoumpos, Constantinos C., Christos D. Malliakas, and Mercouri G. Kanatzidis. "Semiconducting tin and lead iodide perovskites with organic cations: phase transitions, high mobilities, and near-infrared photoluminescent properties." *Inorganic chemistry* 52, no. 15 (2013): 9019-9038.
- [26] K. Markose, Kurias, Manu Shaji, Swasti Bhatia, Pradeep R. Nair, Kachirayil J. Saji, Aldrin Antony, and Madambi K. Jayaraj. "Novel boron-doped p-type Cu_2O thin films as a hole-selective contact in c-Si solar cells." *ACS applied materials & interfaces* 12, no. 11 (2020): 12972-12981.
- [27] Lipomi, Darren J., and Zhenan Bao. "Stretchable, elastic materials and devices for solar energy conversion." *Energy & Environmental Science* 4, no. 9 (2011): 3314-3328.
- [28] Yang, WoonSeok, Byung-Wook Park, EuiHyuk Jung, Nam JoongJeon, Young Chan Kim, Dong Uk Lee, SeongSik Shin et al. "Iodide management in formamidinium-lead-halide-based perovskite layers for efficient solar cells." *Science* 356, no. 6345 (2017): 1376-1379.
- [29] Shih, Yen-Chen, Yu-Bing Lan, Chia-Shuo Li, Hsiao-Chi Hsieh, Leeyih Wang, Chih-I. Wu, and King-Fu Lin. "Amino-acid-induced preferential orientation of perovskite crystals for enhancing interfacial charge

- transfer and photovoltaic performance." *Small* 13, no. 22 (2017): 1604305.
- [30] Gove, H. E., D. Cline, T. M. Cormier, and S. S. Hanna. "The Rochester-Stanford proposal for a search for nuclear isomeric states as candidates for short wavelength lasers." In *AIP Conference Proceedings*, vol. 146, no. 1, pp. 37-39. American Institute of Physics, 1986.
- [31] Bhardwaj, Km Shivani, ShambhaviRai, Sadanand, PoojaLohia, and D. K. Dwivedi. "Investigating the performance of mixed cation mixed halide-based perovskite solar cells using various hole-transport materials by numerical simulation." *Optical and Quantum Electronics* 53 (2021): 1-16.
- [32] Mottakin, M., K. Sobayel, DilipSarkar, HendAlkhamash, Sami Alharthi, KuaananTechato, MdShahiduzzaman, Nowshad Amin, KamaruzzamanSopian, and MdAkhtaruzzaman. "Design and modelling of eco-friendly CH₃NH₃SnI₃-based perovskite solar cells with suitable transport layers." *Energies* 14, no. 21 (2021): 7200.
- [33] DeepthiJayan, K. "Design and Comparative Performance Analysis of High-Efficiency Lead-Based and Lead-Free Perovskite Solar Cells." *physica status solidi (a)* 219, no. 7 (2022): 2100606.
- [34] Omarova, Zhansaya, DarkhanYerezhep, AbdurakhmanAldiyarov, and NurlanTokmoldin. "In silico investigation of the impact of hole-transport layers on the performance of CH₃NH₃SnI₃ perovskite photovoltaic cells." *Crystals* 12, no. 5 (2022): 699.

