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# A Comparison of the Performance of $MAPbI_3$ and $MASnI_3$ as an Inverted Perovskite Structure Using NiO as HTL Through Numerical GPVDM Simulation

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## ABSTRACT

Perovskite solar cells (PSCs) are solar cells that have intriguing characteristics such as environmental friendliness and the capability for high power conversion efficiency, which have attracted study from both scientific investigation and analytical standpoints. However, lead toxicity has become a significant barrier to the widespread use of PSCs. Due to the serious environmental implications of lead, an environmentally compatible perovskite is required. Tin-based perovskite has a considerable impact, showing that it is a good hole extraction material with good mobility and low effective mass. In this study, we explore the impacts of perovskite and hole transporting layer (HTL) thickness, and intensity of light limitations, in inverted PSCs based on the structure of FTO/NiO/$MAPbI_3$/ZnO/Ag and FTO/NiO/$MASnI_3$/ZnO/Ag incorporating GPVDM (General-purpose Photovoltaic Device Model) to evaluate if $MASnI_3$ is a viable substitute to $MAPbI_3$. From the simulation results, the optimized parameters obtained for PCSs under 1 sun incorporating $MASnI_3$ were 27.97%, 0.88 a.u., 0.92 V, and 34.45 mA/cm$^2$. Instead, the optimized parameters obtained for PCSs incorporating $MAPbI_3$ were 24.94%, 0.88 a.u., 0.90 V, and 31.03 mA/cm$^2$. The thickness of the film of both PSC architectures was optimized to provide the best suitable result. The findings show that $MASnI_3$ is employed as a promising perovskite layer in PSCs instead of $MAPbI_3$.

*Keywords*: GPVDM software, $MAPbI_3$, $MASnI_3$, nickel oxide, perovskite solar cells

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## INTRODUCTION

Solar energy offers several distinct benefits over other renewable energy sources, including the worldwide dispersion of sunshine and the decentralized nature of solar energy output (Mohtasham, 2015). Perovskite solar cells (PSCs) have emerged as the "third generation of solar cells," as alternative renewable energy to solve environmental implications such as global warming and greenhouse gases (Ibn-Mohammed et al., 2017). PSCs have been the most recent solar cell type and among the most promising thin-film PV technologies. Strong absorption coefficients, excellent charge carrier mobilities, diffusion duration, and solution processability are the desired properties that make perovskites a potentially new front-runner material for thin-film solar technology (Khadka et al., 2017). These qualities are required for their real implementation in semiconductor-based devices such as solar cells. Sustainable substitutes to present power-generating systems are critical to conserving the planetary environment by ensuring long-term economic prosperity. The recent discovery of halide perovskites as solar energy harvesting and hole-transport materials has contributed to the development of solar technology. Among the several types of PSCs, organic-inorganic metal halide PSCs have garnered substantial interest in recent years due to their high power conversion efficiency (PCE) and ease of fabrication at a cheap cost (Yongjin et al., 2020). The $ABX_3$ perovskite framework is used in organic-inorganic hybrid perovskite substances depending on metal halides. This architecture comprises networks of corner-sharing $BX_6$ octahedra, whereby B is a metal cation (usually $Sn^{2+}$ or $Pb^{2+}$), and X is generally $F^-$, $Cl^-$, $Br^-$, or $I^-$. The A cation is used to equalize the overall charge or to represent a tiny molecular group (Hao et al., 2014). Methylammonium lead tri-iodide ($MAPbI_3$) has often been known to be a perovskite content and is widely employed in PSCs. Even though the efficiencies have now exceeded 20%, long-term stability is the major obstacle to commercializing PSCs on a broader level. As the lead in $MAPbI_3$ is extremely hazardous, industrial applications of $MAPbI_3$-based PSCs are severely limited (Conings et al., 2015; Wang, Phung et al., 2019; Wang, Mujahid et al., 2019), resulting in interest in lead-free PSCs in the sector of solar technologies.

Experts refer to the idea that inorganic halide perovskites, like Sn-, Ag-, Sb-, Bi-, Cu-, and Ge-based solar cells might be employed as lead substitutes (Green et al., 2014; Song et al., 2017). A tin-based perovskite, $MASnI_3$, is a possible option for lead-free PSCs owing to its excellent bandgap of 1.3eV, which are even narrower than $MAPbI_3$ (Baig et al., 2018). It was reported that $MASnI_3$ perovskite has high absorption efficiency with excellent optical features and the broadest light-absorption spectrum compared to $MAPbI_3$ (Du et al., 2016). Sn-based perovskites are environmentally beneficial since they decompose to $SnO_2$ (from $Sn^{4+}$) when exposed to air. Sn-based perovskites and Pb-based perovskites are comparable in their fundamental physical features (Ke & Kanatzidis, 2019; Schileo & Grancini, 2021). Vishnuwaran et al. (2022) have compared the performance of $MASnI_3$

and $FASnI_3$ perovskite materials. Modification in thickness and temperature of the absorber layer revealed that $MASnI_3$ had a higher cell efficiency (23.74%) than $FASnI_3$ (23.11%). Germanium (Ge) is another possible replacement for lead. Recent computational and experimental research has demonstrated that Ge–Sn mixtures are an excellent candidate for enhancing the performance of $Ge^{2+}$-based PSCs. Upon doping a tiny amount (5%) of $Ge^{2+}$ into Ge–Sn mixed halide perovskites, an overall efficiency of 4.48% was attained (Vishnuwaran et al., 2022). The PCE grew to 6.9% after exposure to an $N_2$ environment for 72 hr. Simulation design and investigation of the performance of Sn-Ge-based perovskite in a planar inverter structure yield a PCE of 24.20%, such substantial enhancement established by trap density at the interface layers (Vishnuwaran et al., 2022). Furthermore, Pindolia et al. (2022) proposed an inorganic RbGeI3-based PSC that acquired an efficiency of 10.11% and a greater fill factor (FF) of 63.68% by analyzing alternative inorganic HTL and ETL layers. Like another example of Pb-free PSCs with great promise as light-absorbing perovskite, Cs2TiBr6, and Cs2PtI6 have a good absorption coefficient, a lengthy carrier lifespan, and outstanding stability with adequate bandgaps (1.8 eV and 1.4 eV, respectively). The value can be increased by refining the interface between perovskite and HTL. For this study, $MASnI_3$ was chosen and tested further as a potential replacement for lead-based PSCs.

Aside from the performance of perovskite material, the functionality and maximum efficiencies of PSCs are heavily influenced by the HTL. In the optimization of PSC, HTL can improve the overall performance of PSC by reducing series resistance, enhanced fill factor (FF), and open-circuit voltage ($V_{OC}$) while providing a transport medium for holes to the counter electrode (Yang et al., 2017). Owing to its improved chemical stability, cheap cost, and appropriate energy level, NiO, a direct bandgap inorganic material, has lately caught the scientific community's interest as a viable HTL for stable and efficient PSCs (Hossain et al., 2020). NiO is a significant transition metal oxide that may be easily deposited using a variety of processes, including spray pyrolysis (Danjumma, 2019), sputter deposition (Mulik, 2019), thermal decomposition (Guo et al., 2018), precipitation (Chowdhury et al., 2018), hot-casting (Abzieher et al., 2018), and electrodeposition (Xi et al., 2019). NiO demonstrated good potential in organic solar cells and has a work function of between 5 and 5.6 eV, which satisfies the criteria for an HTL (Nguyen, 2018). NiO, as a p-type semiconductor material, has been effectively used in PSCs with inverted architectures, according to its adequate carrier mobility and good work functionality, which can fit perovskite materials' energy (Chen et al., 2017). The energy band diagram reveals the good positioning of the NiO in such a way as to foster hole extraction from the perovskite material (Nkele et al., 2020). Besides that, there are already many research articles experimentally showing that NiO is a potential material for HTL with good efficiency of 17.75% (Thakur et al., 2020), 19.10% (Mali et al., 2018) and 20.8% (Mahmoudi et al., 2021) which undergone different synthesis processes. In previous work, the General-Objective

Photovoltaic Devices Model (GPVDM) has been used to determine the optimal material parameter for PSCs. GPVDM is a research-leading electrical and optical solver that the electrical transfer characteristics and the optical model pattern of PSCs (MacKenzie, 2016). The PCE of PSC was reported to increase from 9.96 to 12.9% through optimization of the layer thickness using this model (Hima et al., 2018). On the other hand, the effect of the thickness of $MAPbI_3$ as perovskite with Spiro-OMeTAD as HTL and different ETL material ($TiO_2$ and $SiO_2$) has a significant effect on overall PSC efficiency with reported values of 5.6%, 14.5%, and 14.7%, respectively (Mishra & Shukla, 2020; Abdulsalam et al., 2018; Yasodharan et al., 2019). The best-reported efficiencies were obtained with optimal 200 nm and 300 nm ETL thicknesses, respectively. A comparative study on the effect of perovskite layer thickness and charge mobilities in PSCs was also observed with an efficiency of 18.43% (Sittirak et al., 2019). The influence of light intensity has achieved an efficiency from 8.5 to 10%, which indicates that performance can be improved by maximizing the light falling on the solar cell's surface (Mekky, 2020).

There are more solar cell models besides GPVDM that investigate PSC-based structures with $MAPbI_3$, $MASnI_3$, NiO, and ZnO Rahman et al. (2019) used SCAPS-1D to construct a p-i-n structure with three distinct ETL layers ($TiO_2$, ZnO, and $SnO_2$) and compared their properties to that of $MAPbI_3$ as the perovskite layer and NiO as the HTL layer. The research proved that using ZnO as the ETL allowed for the highest possible PCE of 17.84%. The identical model was also used to simulate a $MASnI_3$-based PSC along with NiO as the HTL and PCBM as the ETL to study the details of the device by changing the layer thickness, defect density at junctions, density of states, and metalwork efficiently (Shamna et al., 2020). It is estimated from the simulation result that the designed structure has attained an efficiency of 22.95% with the optimal absorber layer thickness of 600 nm. Another study used the Silvaco ATLAS device model to construct a lead-free titanium PSC ($Cs_2TiBr_6$) using $TiO_2$ as the ETL and comparison of three HTLs (CuPc, $P_3HT$, and NiO), in which NiO gaining the maximum PCE of 8.5% (Samanta et al., 2020). Although the efficiency of $Cs_2TiBr_6$ based-PSC is poor compared to lead-based PSCs, its long-term stability and, most significantly, its eco-friendly nature are predicted to drive it to the forefront of future solar cell application. In addition, Karimi et al. (2020) performed a comparative analysis of the SCAPS and AMPS software applications to explore the impact of ZnO and $SnO_2$ on PSC performances.

Aside from NiO as HTL, many inorganic materials are discovered as HTL layers to study the performance of lead-free PSCs. Anand Kumar Singh et al. (Singh et al., 2021) conducted a simulation study that focuses on $MASnI_3$ perovskite sandwiched between $CuO_2$ as HTL and $TiO_2$ as ETL, achieving maximum efficiency of 27.43% by varying various parameters with the aid of SCAPS-1D simulator. CZTS has recently been analyzed as HTL in tin-based PSC by optimizing layer thickness, energy bandgap, and operating temperature that acquire the best PCE of 20.28% (Reyes et al., 2021). For the first time, the inorganic

material $CuSbS_2$ was employed as HTL in alignment with the $MASnI_3$ as the active layer, and the resulting device achieved an efficiency of 24.1% and further boosting the doping concentration of $MASnI_3$ contributed to an increase in PCE value. (Devi & Mehra, 2019). According to the literature review, inorganic materials are now well-equipped to replace the costly Spiro-MeOTAD and demonstrate the potential to become the ideal alternative for use in the future. Several solvers programs are available, including open source and subscription to model and simulate solar cells. At the same time, certain simulation software shares a common module but varies in terms of speed, features, the quality of the user interfaces, and how easy or difficult to use (Kowsar et al., 2019). It is important to note that this study used an optimized configuration that achieved the highest possible efficiency of 27.43%, the maximum value documented for this configuration by GPVDM simulation software.

From previous work, factors such as the thickness of the film, carrier mobilities, defect density, and light intensity influence device performance optimization. This work investigated the effect of PSCs on the configuration of $MASnI_3$, which was investigated through GPVDM simulations. During the simulations, the thickness of perovskite, the thickness of HTL, and the light intensity were varied to attain the optimal values to maximize the PCE. A comprehensive analysis of the electrical and optical characteristics affecting each performance of $MASnI_3$ and $MAPbI_3$ as perovskite with NiO as HTL has never been described. Furthermore, the results of this inquiry may be extremely valuable and give excellent direction for the understanding of the acquired data, which will aid in revealing the primary processes of PCE rise in the structure of $MASnI_3$ as perovskite and NiO as HTL.

## METHODOLOGY

In Figure 1, the device comprises a layered configuration made from an inverted planar structure (FTO/NiO/Perovskite/ZnO/Ag). Two absorbance layers were compared as the primary carrier producer ($MASnI_3$ and $MAPbI_3$). P-type (HTL = NiO) and n-type (ETL = ZnO) were placed on the top and bottom perovskite layers. The close boundary conditions were applied to the simulation environment, where fluorine tin oxide (FTO) was selected as a glass substrate and silver (Ag) was chosen as the back-electrode layer designated as anode and cathode, respectively. The simulation studies in this work were performed using the GPVDM tool, a freeware solar cell modeling software for photovoltaic systems. The model captures the joint movement of electrons, holes, and transport momentum equation in the orientated area to reflect the movement of loads within the device. The GPVDM software often only provides specialized simulation materials. The NiO, $MAPbI_3$, and $MASnI_3$ material was manually introduced to the GPVDM software following the technique in (MacKenzie, 2016). The absorption and refractive index data of NiO, $MAPbI_3$, and $MASnI_3$ were extracted from the previous work reported by Bakr et al. (2015) and Sun et

al. (2016). This work focuses much on the perovskite and HTL layer, which were largely set to evaluate their effectiveness as active layers.

Both device structure was simulated under one sun AM 1.5G illumination (1 kW/m$^2$; T = 300°K). Table 1 summarizes the designed default GPVDM software variables used during the simulation. The physical parameters of $MAPbI_3$ and $MASnI_3$, such as bandgap (Eg), electron affinity (Xi), density electron states (cm$^{-3}$), density hole states (cm$^{-3}$), electron mobility (cm$^2$/Vs), hole mobility (cm$^2$/Vs) and relative permittivity (Ɛr) were taken from previous experimental and simulation studies (Ahmed et al., 2019; Mohammadi et al., 2021; Hima et al., 2018; Then et al., 2021). Three different approaches were performed to find the optimum parameters of the solar cell, which are (1) different thicknesses of perovskite layer ranging from 50 to 500 nm, (2) different thicknesses of HTL layer varying from 100 to 800 nm, and (3) different values of light intensity. The activated perovskite layer and HTL layer have quite a significant effect on the efficiency of the cells.

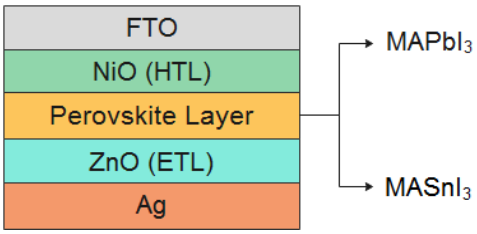



*Figure 1*. Schematic representation of inverted PSCs with $MASnI_3$ and $MAPbI_3$ perovskite material

## RESULTS AND DISCUSSION

Optimization of the perovskite layer thickness is one of the approaches for increasing the PCE. A sufficient thickness is necessary for a successful perovskite device to achieve enough light absorbance and effective charge carrier capture. A perovskite is sufficiently thick in the region of its absorption; then, it leads to an excellent photovoltaic performance (Iakobson et al., 2021; Rai et al., 2020). The thickness of the perovskite film plays an essential part in the device for optimal carrier generation. The influence of perovskite film thickness on cell efficiency was evaluated by computational

Table 1

*Simulation parameter of both perovskite layers and NiO (Ahmed et al., 2019; Du et al., 2016; Hao et al., 2014)*

| No. | Parameters | Layers | | |
|---|---|---|---|---|
| | | $MAPbI_3$ | $MASnI_3$ | NiO |
| 1. | Bandgap energy, Eg (eV) | 1.55 | 1.3 | 1.46 |
| 2. | Electron affinity, Xi (eV) | 3.93 | 4.17 | 3.80 |
| 3. | Density electron states (cm$^{-3}$) | $1.3x10^{26}$ | $1x10^{18}$ | - |
| 4. | Density hole states (cm$^{-3}$) | $9.1x10^{26}$ | $1x10^{18}$ | $1x10^{18}$ |
| 5. | Electron mobility (cm$^2$/Vs) | $2x10^{-1}$ | $2x10^{-2}$ | 2.8 |
| 6. | Hole mobility (cm$^2$/Vs) | $2x10^{-1}$ | $2x10^{-4}$ | 2.8 |
| 7. | Relative permittivity, Ɛr | 6.5 | 8.2 | 11.7 |

models, with a thickness range of 50 to 500 nm (Yasodharan et al., 2019). According to Figures 2(a) and 2(d), the PSC with the $MASnI_3$ has the maximum PCE of 12.88% and $J_{SC}$ of 16.74 ($mA/cm^2$), whereas the PSC with the $MAPbI_3$ has the greatest PCE of 16.96% and $J_{SC}$ of 22.53 ($mA/cm^2$). The higher the thickness of the perovskite layer, the greater the performance of PCE produced.

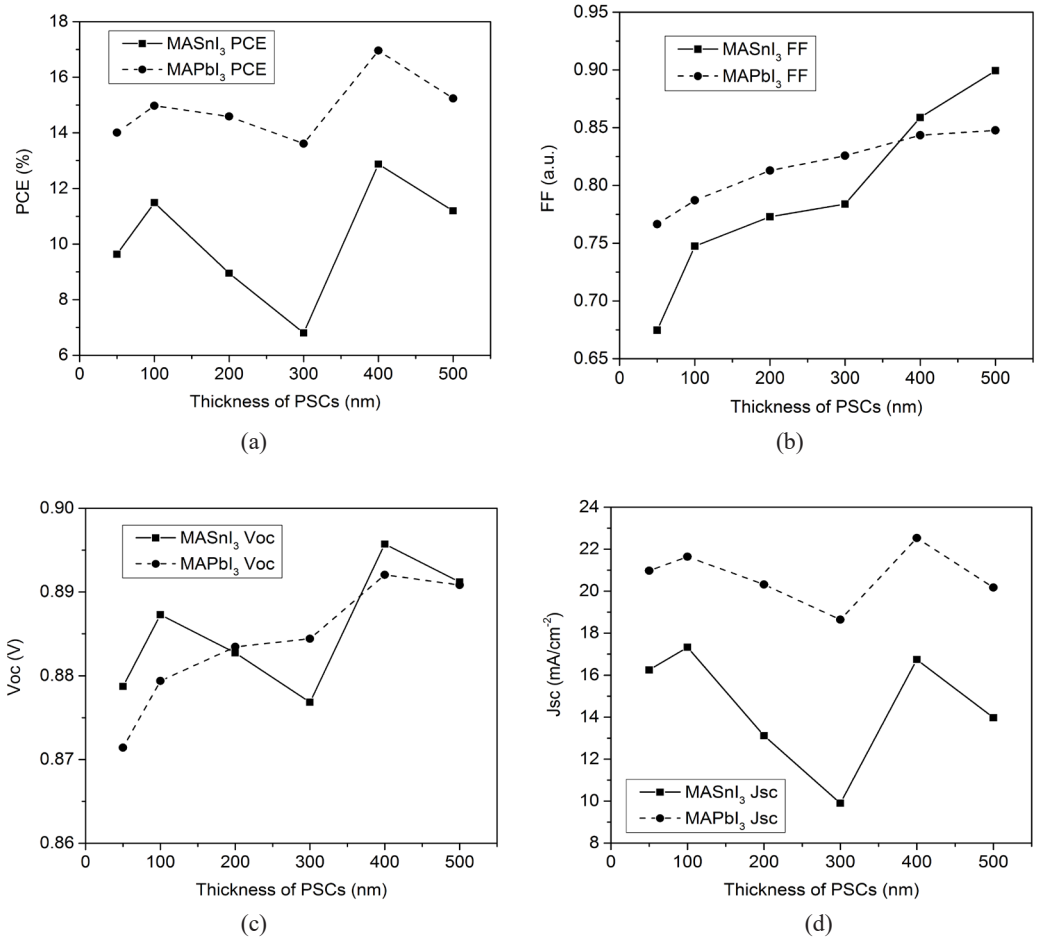



*Figure 2*. The optimized outcome of perovskite thickness generated by the GPVDM software focusing on the comparison between $MASnI_3$ and $MAPbI_3$ produced at 400 nm of (a) PCE, (b) FF, and (c) $V_{OC}$, and (d) $J_{SC}$

The thickness of the perovskite layer increases slowly from 50 to 100 nm, and after that, it decreases when approaching to 200 to 300 nm thickness range. It causes an abrupt drop in the $V_{OC}$ for both perovskite layers (Figure 2c). In contrast, the PCE and $J_{SC}$ showed the highest value at the thickness of 400 nm. It explains how, after the perovskite has reached its ideal thickness, it regulates the interfacial structuring to improve light trapping, resulting in a greater carrier concentration and, as an outcome, a higher $J_{SC}$ (Rai et al., 2020). It is

important to mention that even though the computed $J_{SC}$ for the $MASnI_3$ perovskite device is less efficient than that for the $MAPbI_3$ device, the greatest current density above 15 mA/$cm^2$ can be achieved when integrating $MASnI_3$ perovskite under the bandgap of the 1.30 eV. However, at the thickness of 500 nm, there is also a small significant decrease in PCE and $V_{OC}$. In contrast to PCE and $V_{OC,}$ the outcome of FF keeps increasing with perovskite thicknesses from 50 to 500 nm (Figure 2b). It is due to the thicker perovskite layer that absorbs more significant photons using broader wavelengths, thus increasing the production of electron and hole pairs (Lin et al., 2017).

Although the PCE of $MASnI_3$ is lower compared to $MAPbI_3$, the FF of $MASnI_3$ is larger, which implies lower recombination at the interface. The $V_{OC}$ also constantly increased as the thickness of the perovskite layer increased but dropped when it reached 500 nm, as shown in Figure 2(c). It is also the same case with the simulation study made by Hima et al. (2019), which shows that the PCE drops after the thickness of the perovskite layer reaches the optimal value at 600 nm. As the thickness of the perovskite approached its optimal value, the recombination rate increased, and the efficiency of the cell decreased as a consequence.

In addition, the current simulation study shows much better results than the preceding simulation results using $MAPbI_3$ as a perovskite in GPVDM, which were obtained about 12.83% at 200 nm (Hima et al., 2018) and 14.7% at 300nm (Abdulsalam et al., 2018). Instead, Ahmed et al. (2019) reported that the performance hit as much as 20% at a thickness of 850 nm. A thicker layer of perovskite causes it difficult for charge carriers created by photons to be carried away, reducing the device's effectiveness. This statement also agreed with the report by Nam et al. (2010) about bulk heterojunction organic solar cells and Sievers et al. (2006) regarding polymer bulk-heterojunction solar cells. The optimal thickness should be determined by a balance between the absorption range and the diffusion length of the material (Ragb et al., 2021). Besides that, the obtained result showed higher efficiency than the experimental result of Srivastava et al. (2021), using $MAPbI_3$ perovskite with obtained PCE of 14.44%. Another report also focuses on fabricating $MAPbI_3$ perovskite achieved an efficiency of 14.79% with regulated moisture of 35% in ambient air using a one-step spin coating method (Soucase et al., 2022). In conjunction, solution-processed PSCs based on $MASnI_3$ as the light-absorbing material achieved a PCE of 5.8% (Hao et al., 2014). Based on the analysis between $MAPbI_3$ and $MASnI_3$, the thickness of the perovskite layer plays a major role in increasing the performance of the photovoltaic device (Bag et al., 2020). Additionally, this work obtained efficiency much higher than the experimental outcome, which recently studied NiO nanocrystal film as HTL for Sn-Pb-based PSCs with PCE up to 18.8% (Chen et al., 2021).

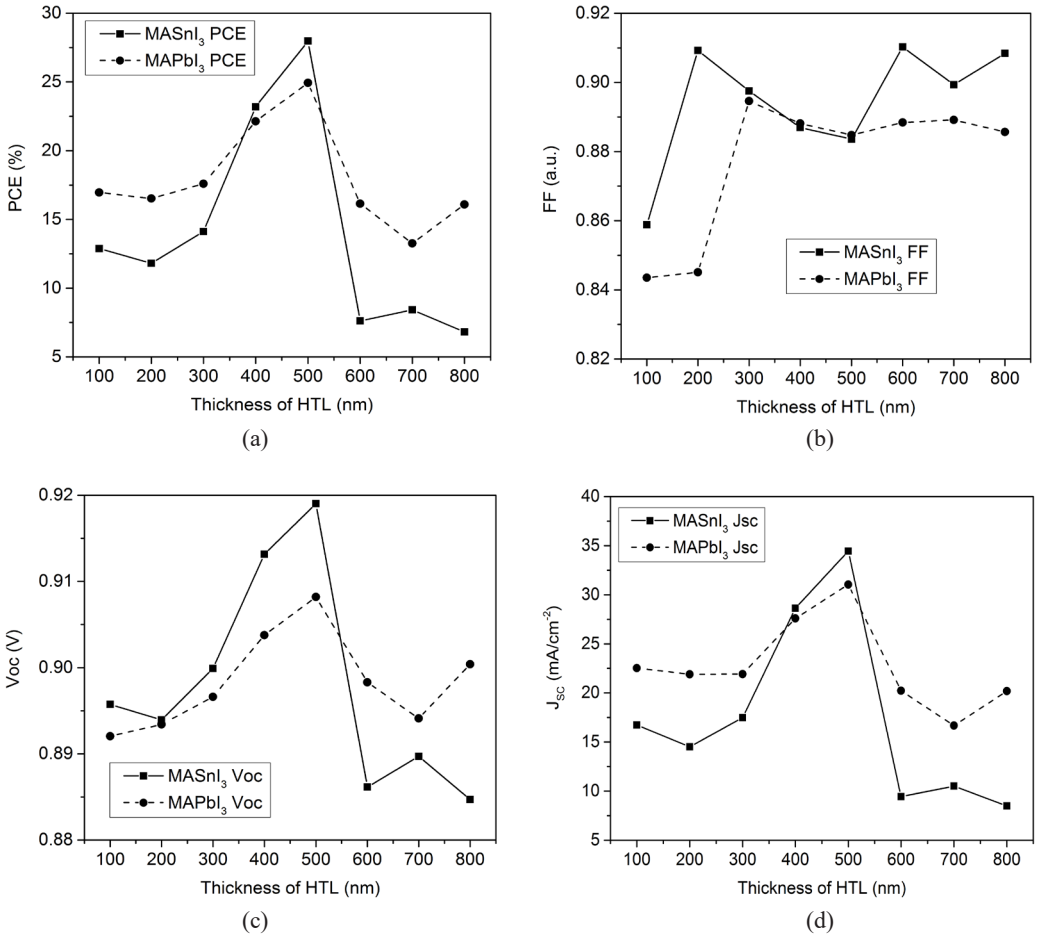



*Figure 3*. The optimized thickness of NiO as HTL generated by the GPVDM software focusing on the comparison of $MASnI_3$ and $MAPbI_3$ obtained at 500 nm of (a) PCE, (b) FF, (c) $V_{OC}$, and (d) $J_{SC}$

Additionally, the impact of light intensity on each solar cell affects all electrical parameters. The quantity of 1 Suns indicates the normal AM1.5 or 1 ($kW/m^2$) lighting on a PSC. Equally, a solar cell system with 10 ($kW/m^2$) could run at 10 suns. The PCE of $MASnI_3$ is much higher than that of $MAPbI_3$, which is at 29.90% and 26.67%, as seen in Figure 4(a). The growing levels of PCE were seen for both materials as the intensity of the light increased up to 10 ($kW/m^2$), which has been previously found in Mekky (2020) utilizing a hybrid perovskite-based solar cell employing a GPVDM model. The above findings indicate that the PCE relies on light-intensity instances and exhibits an extraordinary increase in light-intensity energy transformation. The same trend was also observed in the graph of Figure 4(c); as the intensity of the light increased, the $V_{OC}$ also kept increasing, which is similarly reported by Liu et al. (2017) using $MAPbI_3$ as a perovskite layer.

In contrast, the FF is mainly influenced by the amount of light intensity (Figure 4b). Both structure FF rise when the light intensity is less than 1 kW/m$^2$. However, when the intensity of the light hits more than 1 kW/m$^2$, the FF decreases owing to the impact of series resistance (Mekky, 2020). Figure 4(d) illustrates that the $J_{SC}$ from a solar cell depends linearly on the light intensity, such that a device operating under 10 suns would have 10 times the $J_{SC}$ as the same device under one sun operation. However, this effect does not increase efficiency since the incident power also increases linearly. Instead, the efficiency benefits arise from the dependence of the $V_{OC}$ on short circuits. Subsequently, the same trend of $J_{SC}$ was observed by Kassahun Lewetegn Damena through GPVDM in which the light intensity was varied from 1 sun to 40 suns (Damena, 2019).

The J–V curves of the devices were illustrated in Figure 5, recorded the $MASnI_3$ perovskite-based solid-state device exhibits the highest mean $J_{SC}$ of 32.05 mA/cm$^2$ and

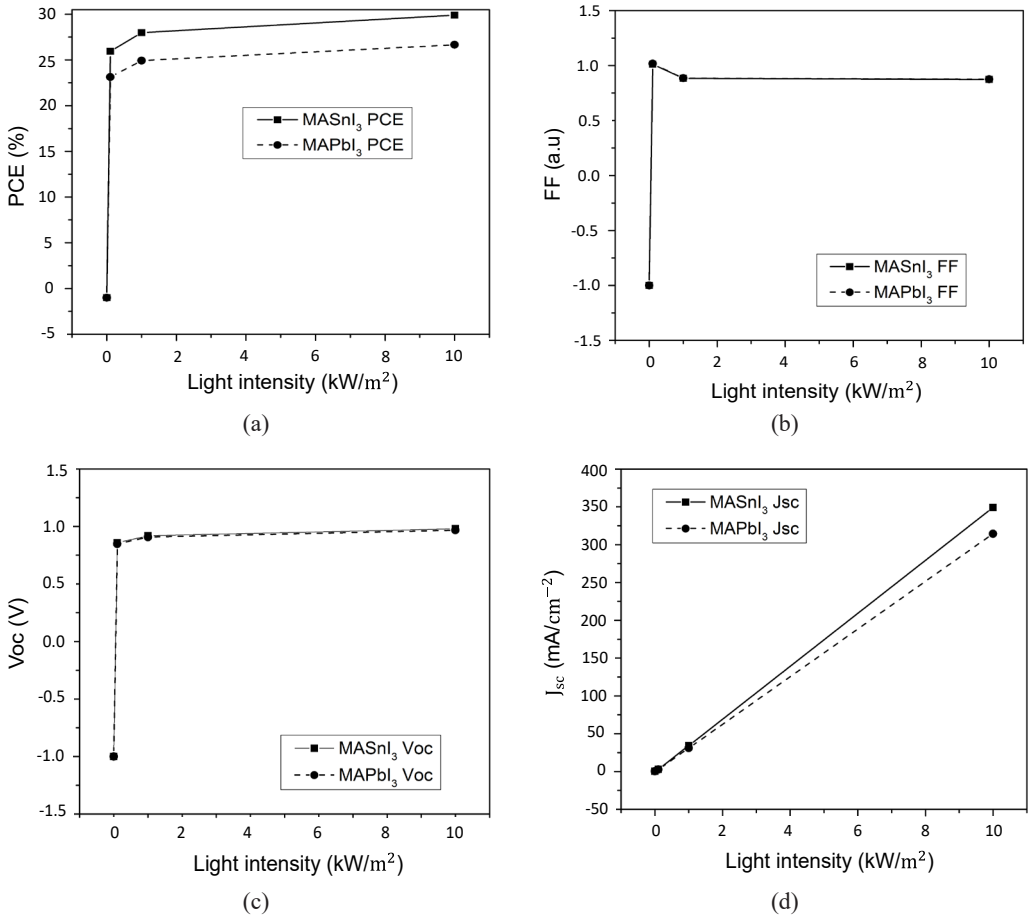



*Figure 4*. The influence of light intensity on $MASnI_3$ and $MAPbI_3$ perovskite achieved an optimum value at 10 (kW/cm$^2$) of (a) PCE, (b) FF, (c)$V_{OC}$, and (d) $J_{SC}$

$V_{OC}$ of 1.6 V under AM 1.5G solar illumination. Meanwhile, the $MAPbI_3$ device showed a slightly lower $J_{SC}$ of 27.93 mA/cm$^2$ and $V_{OC}$ of 1.2 V. A substantial rise in $V_{OC}$ was detected in the $MASnI_3$ device compared to the $MAPbI_3$ device. The current analysis also demonstrates the potential ability of tin-based perovskite contrasted with lead-based perovskite. Previously, Mandadapu et al. (2017) presented a simulation regarding $MASnI_3$ PSC with the thickness of 600 nm obtained PCE, $J_{SC}$, and $V_{OC}$ of 24.82 %, 25.67 mA/cm$^2$ and 1.04 V correspondingly. Nevertheless, another simulation study of $MASnI_3$ compared to $MAPbI_3$ reported by Shyma and Sellappan (2021) gained an efficiency of 24.3 % with $J_{SC}$ of 32.30 mA/cm$^2$, which is higher than the current study yet still shows a lower $V_{OC}$ of 1.2 V. Regardless of the simulation studies, Li et al. (2019) demonstrated an experimental result of $MASnI_3$ developed using a two-step technique for the deposition of solid and homogeneous perovskite layers, reaching the optimum value of PCE at 7.13 %, $J_{SC}$ at 22.91 mA/cm$^2$ and $V_{OC}$ at 0.486 V.

It is well known that the present simulation result of $MASnI_3$ PSC has enhanced the photovoltaic performances of the devices compared to the $MAPbI_3$ PSC. It can be supported by the fact that by integrating the AM 1.5G solar spectrum below the bandgap of $MASnI_3$ (1.30 eV) perovskite, the greatest current density that can be produced, despite the lower $J_{SC}$ found for $MAPbI_3$ perovskite (Hao et al., 2014). Besides that, this could be owing to the perovskite's wide optical absorbance cross-section and the well-developed interstitial pore opening by the hole conductor, which allowed for this tremendous current density produced by $MASnI_3$ (Cao & Yan, 2021; Du et al., 2016). Additionally, the insertion of the NiO HTL in the structure significantly improves the PCE of the solar cells, which is attributed due to the suitable band alignment of the NiO and perovskite.

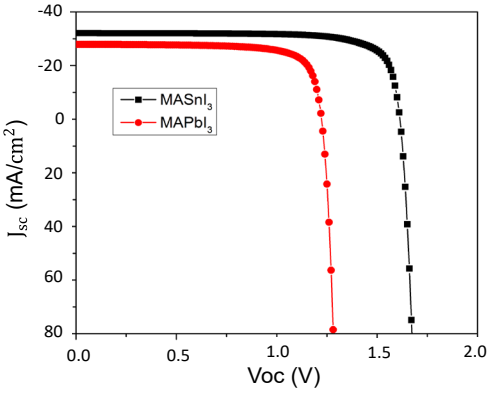
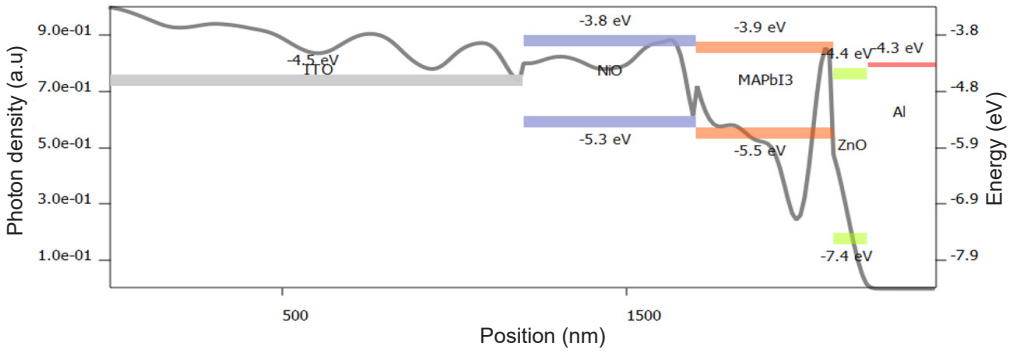



*Figure 5*. The optimized curve of photocurrent density-voltage (J-V) achieved higher by $MASnI_3$ at $J_{SC}$ of 32.05 mA/cm$^2$ and $V_{OC}$ of 1.6 V in parallel with $MAPbI_3$ obtained at $J_{SC}$ of 27.93 mA/cm$^2$ and $V_{OC}$ of 1.2 V as perovskite

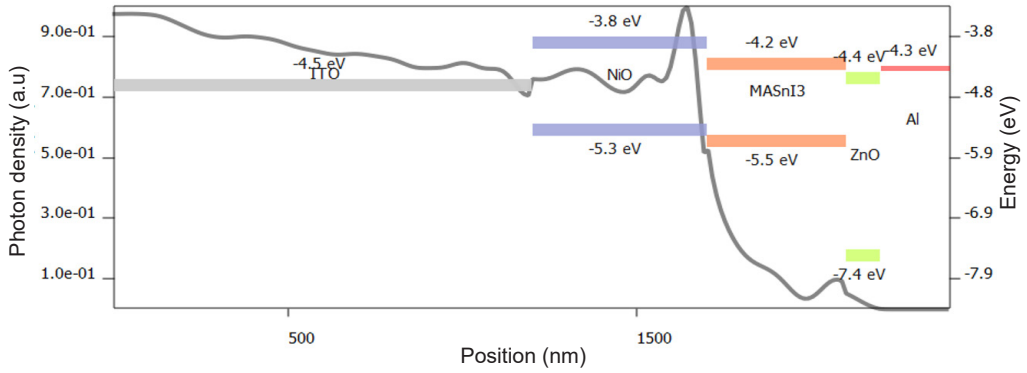
The photon density distribution corresponding wavelength as a function of the position of the $MAPbI_3$ device layers was presented in Figure 6(a). Most photons are absorbed in the perovskite absorbance layer. Therefore, massive electrons and holes have promoted the device's efficiency (Said & Woon, 2019). The same trend was also observed for the $MASnI_3$ PSC in Figure 6(b). The photon of both PSCs was more significant from FTO and decreased after the Ag electrode was incorporated. When the light penetrates an absorber layer of the film, the process of pumping electrons through the valence band into the conduction band

occurs. The electrons quickly start to move to the ETL of the n-type ZnO, whereas the holes begin to migrate to the HTL of the p-type NiO. The ZnO has a lower work function (−4.4 eV) which matches with the lowest unoccupied molecular orbital (LUMO) energy level of $MAPbI_3$ perovskite film (LUMO = −3.9 eV) and $MASnI_3$ perovskite film (LUMO = −4.2 eV). The band structure of perovskite/ZnO further accelerates the electron transport to the Ag cathode (LUMO = −4.3 eV). NiO work function (-5.3 eV) must be aligned as closely as possible with the highest molecular orbital (HOMO) energy level of the ITO (HOMO = −4.0 eV) to deliver accurate hole direction. The minority and majority carriers are generated when a photon is absorbed. Absorbed photons at the HTL interface (NiO) showed that the $MASnI_3$ structure absorbs higher than the $MAPbI_3$ structure but decreases in time. It indicates that the stored charge at the hole-extracting interface of NiO could have a strong downward band bending on the perovskite side at the perovskite/HTL interface (Ravishankar et al., 2019). It is consistent with that tin-based perovskite produces the highest efficiency levels. The resulting shift of NiO in the work function leads to a more beneficial energy level alignment with the $MASnI_3$ perovskite, which is believed to facilitate charge extraction. Therefore, the photovoltaic performance is enhanced by an appropriate work function in relation to the perovskite interfaces. The downward band bending is potentially detrimental to charge extract and recombination kinetics because it sends holes back to the perovskite surface, which could increase the device's performance. The driving energy for hole injection happens from the valence band maximum of the HTL and should be greater in energy than the valence band maximum of the perovskite (Haider et al., 2022).

However, the photon density produced at the $MAPbI_3$ interface is higher than at the $MASnI_3$ interface. The $MAPbI_3$ perovskites have much higher radiative recombination coefficients, leading to the situation that $MASnI_3$ is much less charge carrier densities faced in photovoltaic at intensities around 1 sun (Kirchartz, 2019). Therefore, only a small percentage of photons will be created within the interface of $MASnI_3$.




(a)




(b)

*Figure 6*. Photon density distributions (a) $MAPbI_3$ and (b) $MASnI_3$ as perovskite with the AM 1.5G solar spectrum interfaced with the thickness of the device

## CONCLUSION

In summary, tin-based perovskites have excellent optoelectronic properties which lead to a promising candidate for efficient lead-free PSCs. Under 1 sun light intensity the tin-based perovskites have achieved the highest PCE of 27.97% while the lead-based perovskite achieved PCE at 24.94% using GPVDM software. During the optimization of perovskite layer thickness both perovskite material found at 400 nm in which the higher efficiency was attained by lead-based perovskite. Nevertheless, after the evaluation made on the HTL thickness the highest efficiency was noticed on tin-based perovskites at 500 nm with high $J_{SC}$ and $V_{OC}$ value. The findings imply that lead-free $MASnI_3$ has a huge potential as an absorber layer when combined with a robust inorganic hole transport material like NiO. Moreover, further increase of light intensity in each structure implies a progressive increase in PCE. Encouragingly, simulation models produced a maximum PCE of more than 20% that can be achieved from tin-based PSCs under optimized conditions. A deeper study on the previous simulation and experimental of each of the photovoltaic parameters such as PCE, $J_{SC}$, $V_{OC,}$ and FF reveals that the Sn-based devices perform better for high efficiency in lead-free PSC. In comparison to, lead-based counterparts, tin-based PSCs have a higher $V_{OC}$ with a record value of 1.6 V, which consider higher than previous studies. Importantly, these computational results demonstrate that the absorber and HTL layers significantly impact system efficiency. The construction of a high-efficiency tin-based PSCs will be aided by this simulation study.

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