

The Effect of Active Layer Thickness on the Performance of Tin Halide Perovskite ($\text{CH}_3\text{NH}_3\text{SnI}_3$)

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Abstract

The effect of active layer thickness on the electrical properties of Tin Halide Perovskite ($\text{CH}_3\text{NH}_3\text{SnI}_3$) was studied using the General-purpose Photovoltaic Device Model (GPVDM) software which is an efficient tool in simulating optoelectronic devices. The simulation was based on some semi-empirical results, and the parameters were inputted to definite materials of each active layer of the solar cell while parameters such as operational temperature and suggestive resistance were based on default entry of the GPVDM simulation software. Absorber thickness was varied from 100nm to 1000nm while other parameters were kept constant. Optimum efficiency of 13.9% was obtained by absorber layer with 600nm thickness, with fill factor and open circuit voltage values decreasing as the absorber thickness increases. Results also showed that the efficiency of this device can be improved by adjusting the active layer thickness.

Keywords: GPVDM software, Organic solar cells, Perovskites, Absorber thickness

Article History:

Received 22 February 2021

Received in revised form 01 June 2021

Accepted for publication 20 June 2021

Published 07 July 2021

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1. Introduction

Today's energy landscape is dominated by the use of fossil fuels which generate harmful pollutants to the atmosphere and this is a major cause of global warming. Research has also showed that the fossil fuel reserves are depleting and will soon run out [1]. In order to address the growing demand for clean and renewable energy, it is pertinent to advance innovative research in renewable and sustainable alternatives to existing fossil fuel technologies. Photovoltaic (PV) is a promising energy generating technology that harnesses solar energy and has the potential to mitigate greenhouse gas emission. As a result, researchers are focused on the optimization of both organic and inorganic PV cells structure, transparent conducting layer, absorber layer, as well as conversion efficiencies and lifetime

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respectively [2].

The perovskites solar cells are among the emerging PV technologies and have recently attracted intense attention, owing to remarkable improvements in performance resulting from continued research and investigation of new materials composition, new device architectures, and improved fabrication processes [2], [3], [4]. Perovskite is a common name for compounds whose composition is characterized by the chemical formula ABX_3 in which A and B are cationic species with different size and X is an anionic specie [5]. The key merit of perovskite solar cells is the possibility of fabricating solar modules from solution processing techniques thereby reducing cost and energy payback time. Other advantages include huge availability of material, flexibility on substrates and easy sample preparation [6]. However, the drawbacks on this class of solar device include perovskite sensitivity to moisture, health implication due to the presence of lead in the mostly recorded efficient structures [7], low lifetime due to phase transition and a few others.

There has been an increasing interest in perovskite solar cells in the last few years which has seen it record growth in efficiency from as little as 3.8% in 2009 to more than 22% in 2014 [7], [8], making it the fastest advancing solar PV technology. Modern and leading perovskite structure are based on a transparent conducting oxide/ETL/Perovskite/HTL/metal structure, where ETL and HTL refer to electron-transport and hole-transport layers respectively [9]. Not only are research efforts aimed at understanding and optimization of the energy levels and interactions of different materials at these interfaces but also efforts are targeted at addressing challenges of film quality and thickness during device fabrication. The light-harvesting (active) perovskite layer of the solar cell have been shown to impact the performance of the solar cell. Utilizing the General Purpose Photovoltaic Device Model (GPVDM) software, [10] simulated different thickness of P3HT-PCBM blend as photoactive layer, with indium tin oxide (ITO), PEDOT:PSS and aluminum (Al) as front electrode, electron blocking layer and back electrode respectively, showed how strongly the variation in active layer thickness affected the electrical performance. Similarly, [11] used the GPVDM software to investigate the effect of thickness and temperature on the performance of perovskite solar cell having ($CH_3NH_3PbI_3$) as its active layer. The optimal active layer thickness was found to be 3×10^{-7} m with an efficiency of 14.7% while the optimal temperature was found to be 300 K with power conversion efficiency of 15.4%.

A comparative study of lead-free perovskite solar cell using different hole transport materials was carried out by [12] after developing a Tin-based perovskite simulated model and designing the novel perovskite based architecture TCO/Buffer (TiO_2)/Perovskite/Hole Transport Material (HTM). The set up was analyzed using the solar cell capacitance simulator (SCAPS-1D). Results obtained showed that lead-free ($CH_3NH_3SnI_3$) has great potential to be an absorber layer with suitable inorganic HTMs like CuI (PCE 23.74%), CuO_2 (PCE 19.17%) and organic HTMs like Spiro-OMETAD (PCE 23.76%) and PTAA (PCE 23.74%). Influence of perovskite thickness and the doping concentration on the solar cell performance were also investigated.

Furthermore, [13] in their study of n-i-p perovskite solar cell (FTO/ITO/Perovskite/PEDOT: PSS/Au) using SCAPS simulator demonstrated improved cell performance by optimizing the absorber thickness to $1 \mu m$. They further showed that adopting ZnO and TiO_2 as ETL and Copper (I) thiocyanate ($CuSCN$) as HTL resulted in enhanced power conversion efficiency of 25.02%. However, defect at the perovskite/ TiO_2 interface was reported which was found to have an undesirable effect on the solar cell performance.

In this work, we utilized the GPVDM simulation software to determine the optimal thickness of perovskite solar cell absorber active layer ($CH_3NH_3SnI_3$) for improved device performance.

2. Device Structure

In this work, we adopted a perovskite solar cell with p-i-n planar device architecture based on ITO/PEDOT:PSS /($CH_3NH_3SnI_3$) /ZnOAl; Poly (3,4-ethylenedioxythiophene): Polystyrene sulfonate (PEDOT:PSS) as a hole transport layer (HTL) and Zinc Oxide (ZnO) as an electron transport layer. Indium Tin Oxide (ITO) have been selected as the transparent conducting oxide (TCO) while Aluminum is chosen as the back electrode for charge extraction. A

graphical representation of the planar architecture for the PSC model is depicted in Figure 1.

3. Method

We input parameters to definite material of each active layer of the solar cell. Some parameters for the simulation are based on experimental results and are properly captured in Table 1. While other optimal and suggestive parasitic resistances are based on the default entry of the GPVDM simulation software. We varied the absorber thickness from 100 nm to 1000 nm in steps of 100 nm while keeping other parameters invariable in other to determine the absorber thickness that gives the higher efficiency. For each simulation, we also displays different light absorption profile. For the electrical parameters calculation we used 1cm^2 of the device for 1.5G illumination.

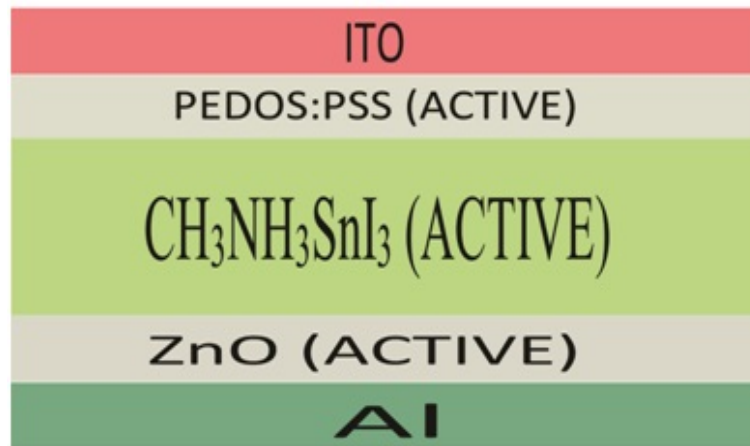


Figure 1. A sketch of the simulated perovskite structure

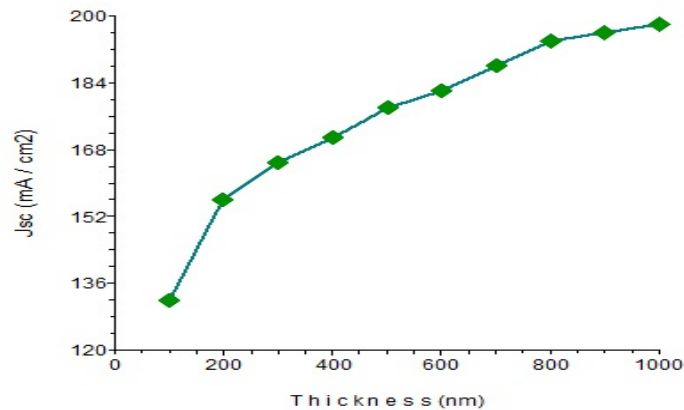


Figure 2. Short circuit current versus absorber thickness

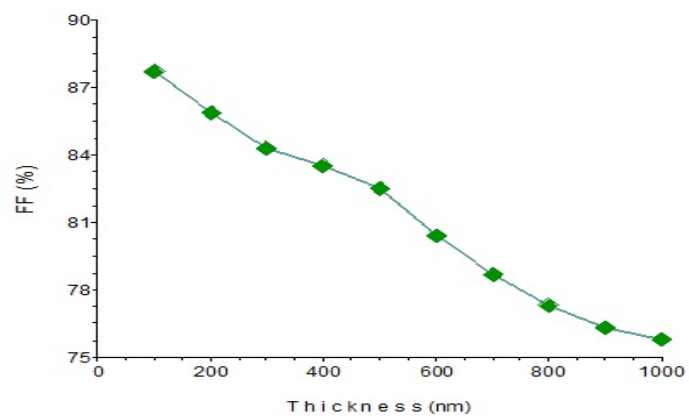


Figure 3. Fill factor versus absorber thickness

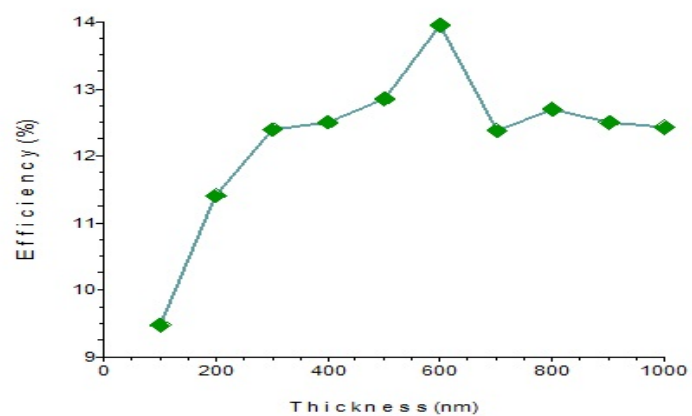


Figure 4. Efficiency versus absorber thickness

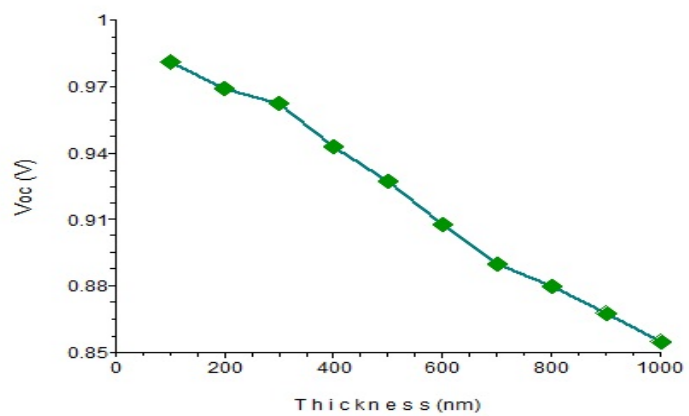


Figure 5. Open circuit voltage versus absorber thickness

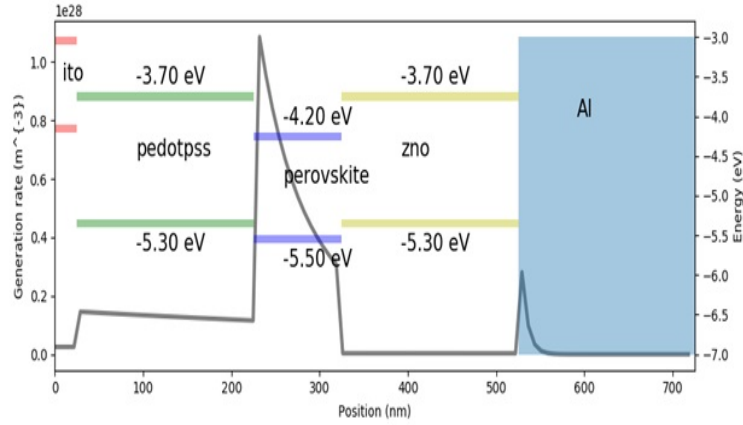


Figure 6. Generation rate profiles in individual layers with absorber thickness of 100 nm

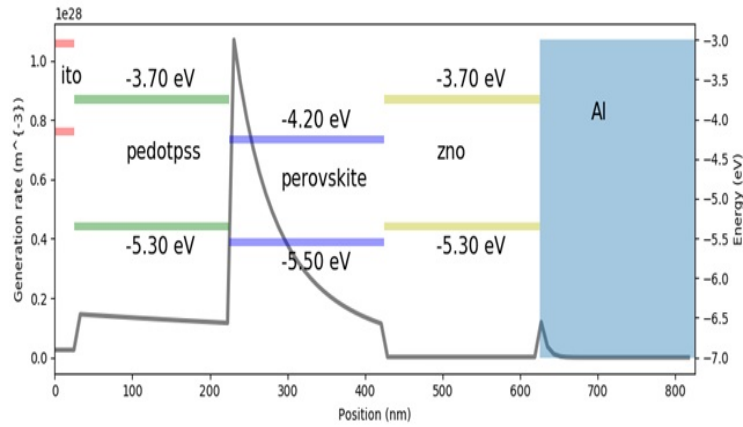


Figure 7. Generation rate profiles in individual layers with absorber thickness of 200 nm

Table 1. Simulation parameters

Material Properties	$CH_3NH_3SnI_3$	PEDOT:PSS	Zinc Oxide
Thickness (nm)	Varied	1.50	2.0
Bandgap (eV)	1.30	1.6	1.6
Electron Affinity (eV)	4.20	2.1	4.3
Relative Permittivity	10	3	9
Electron and Hole Mobility $m^2 V^{-1} S^{-1}$	1.6×10^{-3}	10^{-4}	$1.0 \times 10^{-1} / 2.5 \times 10^{-1}$

Simulation parameters adopted from; [12], [13], [14] were utilized.

4. Results and Discussion

Figure 2 above shows that J_{sc} values increases with increasing thickness, this is because at higher thickness more photons are generated which eventually leads to more generation of electron-hole pair. The obtained results shows similar progression with those achieved by [15].

Figure 3 shows decrease in FF values which is in agreement with reports of [12] for simulated $CH_3NH_3PbI_3$

based cells. The reduction in FF is attributed to high rates of recombination as absorber layer increases and can also be attributed to larger distance between the electrode resulting in smaller electric field [16].

Figure 4 above shows that as the thickness of $\text{CH}_3\text{NH}_3\text{SnI}_3$ is increased, the efficiency of the solar cell increases up to maximum at 600 nm thickness (13.9%), further increase of absorber thickness from this point leads to decrease in efficiency.

As noted from figure 5, that the increase in recombination level as thickness increases invariably leads to decline in V_{oc} .

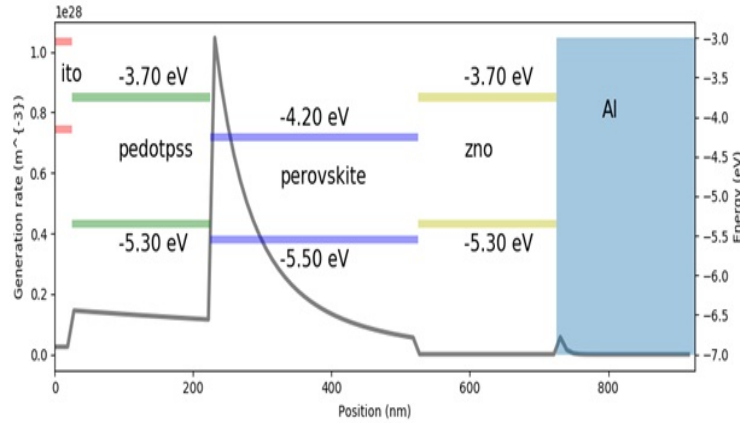


Figure 8. Generation rate profiles in individual layers with absorber thickness of 300 nm

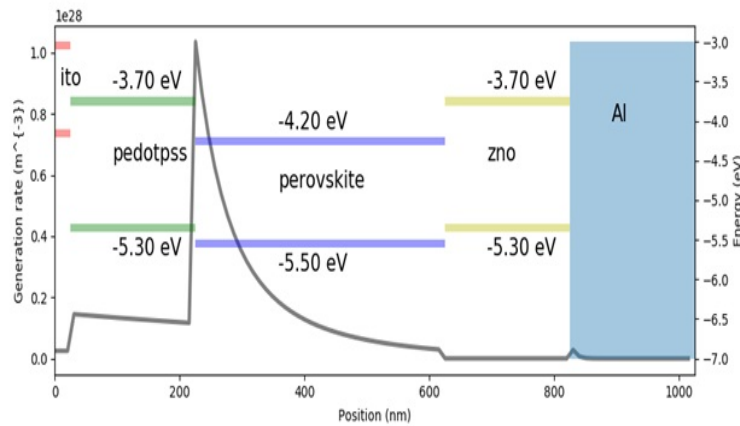


Figure 9. Generation rate profiles in individual layers with absorber thickness of 400 nm

The spectral absorption is important in determining how and where absorbed photons are converted into photo-generated charged and hence the current produced in the solar cell. Individual layers can absorb and convert photons into photo-generated carriers based on the availability of different incident energy photons as shown in figures 6 to 15. For each profile, there is little or no significant generation rate at the ITO/PEDOT:PSS interface. While at the PEDOT/ $\text{CH}_3\text{NH}_3\text{SnI}_3$ interface, a sharp decrease of photon generation rate is observed showing a significant rate of photon conversion into electron-hole pair for all range of thickness. This significant photon conversion rate is attributed to both the PEDOT:PSS which also take part in absorbing selective energy photons [17], [18], and large exciton density in perovskite material which accounts for the ease in photo-current generation. It is important to state that for thinner absorber length as can be seen in figures 6 and 7, the degree of decrease is sharp as compared to

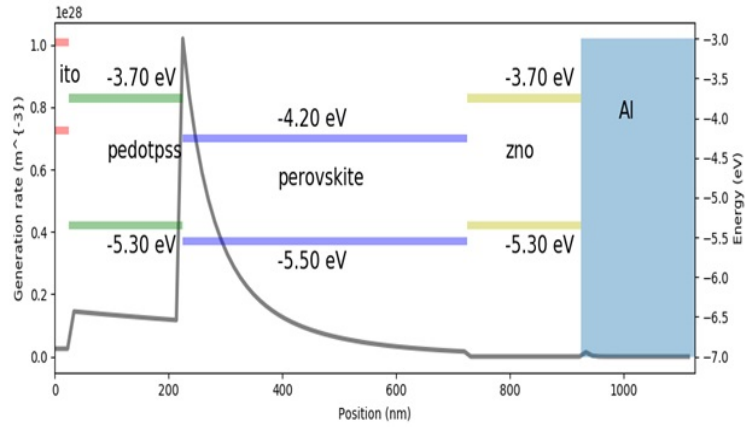


Figure 10. Generation rate profiles in individual layers with absorber thickness of 500 nm

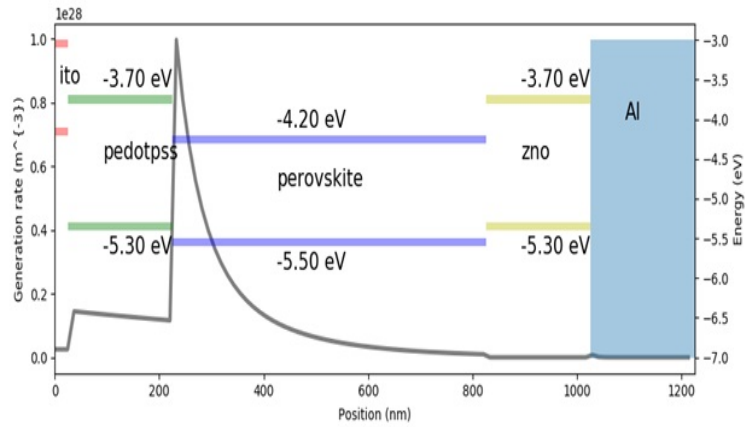


Figure 11. Generation rate profiles in individual layers with absorber thickness of 600 nm

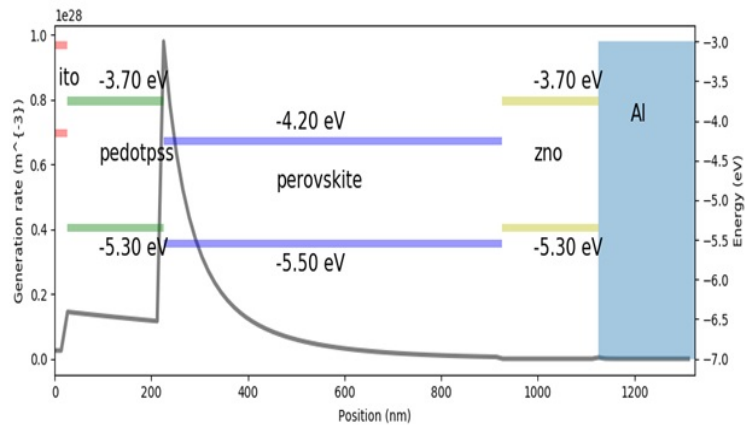


Figure 12. Generation rate profiles in individual layers with absorber thickness of 700 nm

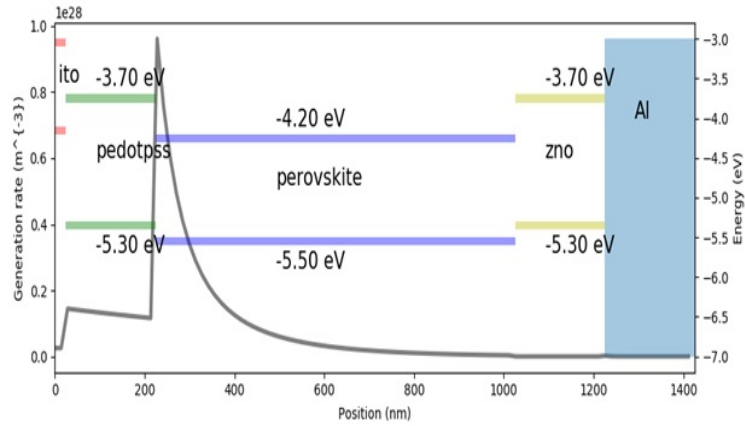


Figure 13. Generation rate profiles in individual layers with absorber thickness of 800 nm

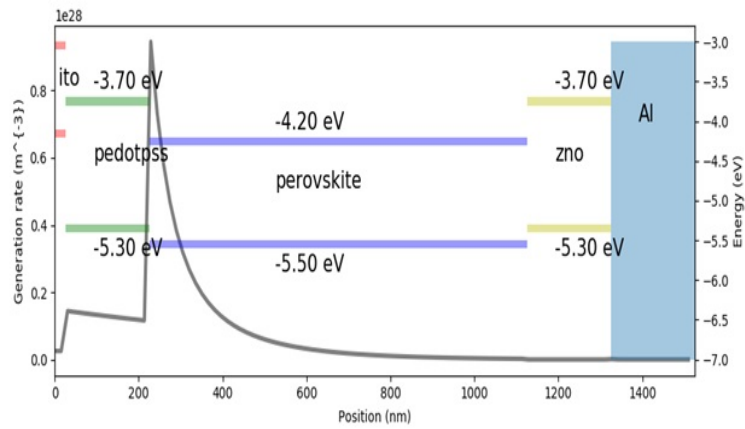


Figure 14. Generation rate profiles in individual layers with absorber thickness of 900 nm

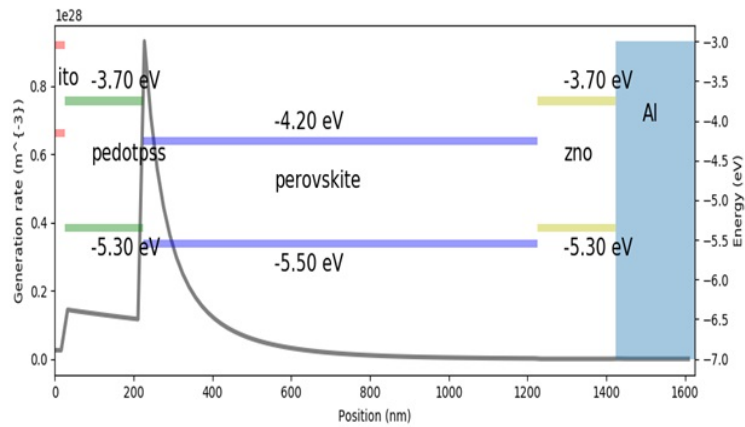


Figure 15. Generation rate profiles in individual layers with absorber thickness of 1000 nm

more elongated decrease in the generation profile with thicker absorber lengths (from figures 8 to 15). No photo-current generation is observed at the $CH_3NH_3SnI_3/ZnO$ interface for all range of absorber thickness. Furthermore, we observe from the spectral distribution profile that ZnO/Al interface produces a significant photo-generated based on suitable band-edge position figures 6 and 7, but this diminishes with increasing absorber thickness (figure 15). At the end, unabsorbed photons exit the device at the Al side in the form of transmitted/unutilized energy. The spectral distribution are similar to those obtained by [13].

5. Conclusion

In this work, $CH_3NH_3SnI_3$ peovskite device efficiency was analyzed using GPVDM solar cell simulation software. The device efficiency analysis indicates an increasing efficiency of up to 13.9% (optimal efficiency) at 600 nm thickness. It also shows that optimum active layer thickness improves the overall device performance. Additionally, the findings shows a considerable improvement in efficiency compared to more stabled, and recently investigated $CH_3NH_3PbI_3$ perovskites. Further efficiency enhancement can be realized by tuning other layer thickness within the cell or by changing the device structure and materials.

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