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Spectral Distribution Profiles of Absorbed And Transmitted Photons In Perovskite Solar Cell: Influence of Active Layer Thickness

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Abstract

Utilization of incident photons in any functional photoelectric device like solar cellsis one of the crucial phenomena which help in deciding its power conversion efficiency. In this study, different active layers in a typical perovskite solar cell (PSC) have been modified to trace the spectral profiles of absorbed and/or transmitted photons in/through the device. Standard light source (AM 1.5G) was considered for developing wavelength dependent absorption and transmittance profiles of individual layers of PSC. At the same time, thicknesses of all active layers have been modified to check the feasibility of effective photon absorption for the optimum performance as energy conversion device. In the present work, PSC was constructed of poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS), perovskite and zinc oxide (ZnO) active layers along withsuitable front and back metal contacts.Through this analytical simulation study, experimentalists will get benefitted in designing/implementing their resources towards advancement of PSC research.

Keywords: Perovskite, PEDOT:PSS, ZnO, absorption, transmittance

1. Introduction

Modelling and simulation of various functional photoelectric devices is one of the trending fields of research in past decades. Since many years, computational physicists have provided an ampleamount of theoretical suggestions and future strategies to the wide research community.Among all photoelectric devices, solar cells have gained much attention due to high energy demand and green route for energy generation. Different solar photovoltaic technologies like crystalline silicon (Si), a-Si, CdTe, CIGS, dye sensitized solar cell (DSSC), organic solar cells (OSC) [1, 2, 3], polymer solar cells [4, 5], perovskite solar cells (PSC) [6,7] and generic solar cells [8, 9, 10]have been explored both, theoretically and experimentally. Recently, perovskite based solar cells have shown tremendous potential and hence advancement in the realization of high efficient solar energy conversion devices. However, in spite of being potentially viable technology, PSC is struggling a lot in large scale applications. Moderate to poor device stability and low transparency are few of the limiting factors behind leisurelieracceptance of PSCs. Many researchers have examined theoretical properties of different solar cell technologies with the help ofdevice level simulation. However, a few studies have been reported which considered and accounted individual photons while they pass through thedevice either utilised or unutilised.

In the present work, we have made efforts to pinpoint mainly on the distribution of number of photons (of certain energy) get absorbed and transmitted in PSC which ultimately affects the efficiency of any solar cell. In addition, we have gained crucial insights on photon utilization for three different PSCs under identical simulation conditions. Briefly, effects of individual active layers' thicknesses in typical PSCs have been discussed with spectral profiles.

2. Perovskite solar cell configuration

Perovskite solar cell consisted of poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS)as a hole transport layer (HTL) and zinc oxide (ZnO) as an electron transport layer (ETL) was adopted for the present study. Fig-1 shows a typical device configuration of perovskite solar cell with three active layers and appropriate metal contacts for the collection of photogenerated charge carriers. Three different devices named PSC-1, PSC-2 and PSC-3 have been considered for the comparative analysis based on device simulations. Thicknesses of different active layers and metallization in each of these PSCs can be referred from Table-1.

3. Device simulation

A standard AM 1.5G was used as a light source which was allowed to enter in the device from ITO side for the simulation purpose.Each configuration was simulated with the help of gpvdm software to acquire the absorption, generation and transmittance of monochrome photon. Spectral range from 350 to 750 nm has been selected for improving the accuracy of the data (through number of max iterations) and shortening the simulation time. Applied voltage range was tuned from 0 to 1.25 V to get the quantitative information about the photogenerated carriers which ultimatelydecide thenumber density of photons across the device. Optimal values of parasitic resistances were accepted as default from simulation tool. Resulted output in the form of images has been recorded and presented to compare the optical characteristics of PSC-1, PSC-2 and PSC-3.Consequential discussion and visualization of individual photon (of particular energy) have been described in the following section.

ISSN: 0971-1260
Vol-22-Issue-16-August-2019

4. Results and discussion

As discussed in the preceding section, wavelength range of 350-750 nm wasintended to scrutinizefor ‘absorbed’ and ‘transmitted’ behaviour of photons across the device. Thus, the output of the simulation was limited to this spectral range and presented in the form of distribution of available and absorbed photons. Fig-2 shows the spectral distribution of available photons while travelling through different active/absorbing layers in each PSCs. As it can be seen from Fig-2 (a), (b) and (c), PEDOT:PSS layer get exposed to different number of photons from 350 to 750 nm. Particularly, number of photons having wavelength less than 400 nm is noticeably lesser than the photons of 450 to 750 nm.Based on availability of different incident energy photons, individual layers may absorb and convert in photogenerated carriers. The ability of either absorption or conversion solely depends on the material aspects. Profiles of successfully absorbed photons in devices PSC-1, PSC-2 and PSC-3 have been presented in Fig-3 (a), (b) and (c), respectively. It is worth noticing here that visual difference in the profiles is only due to different thickness of the layers. Importantly, number of absorbed photons remainsequal in any selected layer at presumed depth and the point of interest.Photo conversion from such unique point of interest greatly depends on the number of successfully absorbed photons. Moreover, a number density of available photons which is being passed though the layer can be influenced by(1) absorbed photons in all previous/same layer/s, (2) successful conversion of photons into the free carriers in all previous layers and (3) reflected photons from the ITO surface. Profiles of number density of available photons between end-to-end of each PSCs are presented in Fig-4. As can be seen clearly from the figure, the number of photons get decreased sharply at PEDOT:PSS/Pervoskiteinterface showing high rate of conversion of photons into photogenerated carriers (electrons and holes). Noteworthy, PEDOT:PSS which was believed to be HTL only, also take part in absorbing selective energy photons. It is interesting to note that remaining photons get utilized at ZnO/Al interface and produce photogenerated electron-hole pairs based on suitable band-edge positions. At the end, left over photons that couldn’t get either absorbed or converted into the electron-hole pairs come out of the device (from Al side) in the form of transmittedphotons (unutilized energy). Fig-5 shows the distribution of such kind of transmitted photons for individual PSCs under study. As it can be easily observed from Fig-5 (a) and (b), PSC-1 and PSC-2 behave almost same as far as amount of unutilized light is concerned. However, PSC-3 showed orders of difference in transmitting left-out photons. Detailed analysis of photo

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conversion from each of the device may lead us to find most suitable PSC configuration facilitating optimal power conversion at cost effective manner.

5. Conclusion

In conclusion, through this analytical simulation of perovskite based solar cellswe have found out the role of individual layer thickness on overall photoabsorption and transmittance. Spectral profiles which were obtained by simulating PSCs under standard test conditions gave insight into the device's ability to utilise different energy photons. Such theoretical study will enlighten a pathway for research community to design and fabricate highly efficient nano-photonic devices.

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Table 1 Layer thickness in each solar cell

	Thickness (nm)		
	PSC-1	PSC-2	PSC-3
ITO	25	25	25
PEDOT:PSS	200	100	50
Perovskite	400	200	200
ZnO	200	100	50
Al	200	200	50
Total	1025	625	375

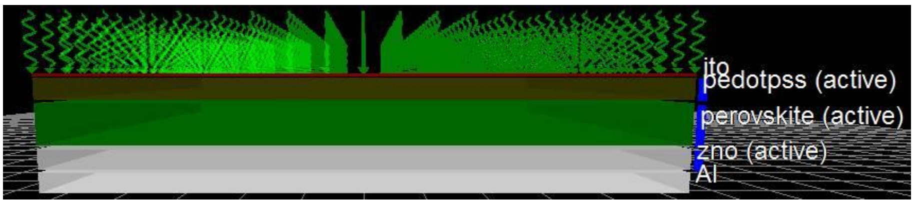

Figure 1 Device cross sectionalschematic

ISSN: 0971-1260
Vol-22-Issue-16-August-2019

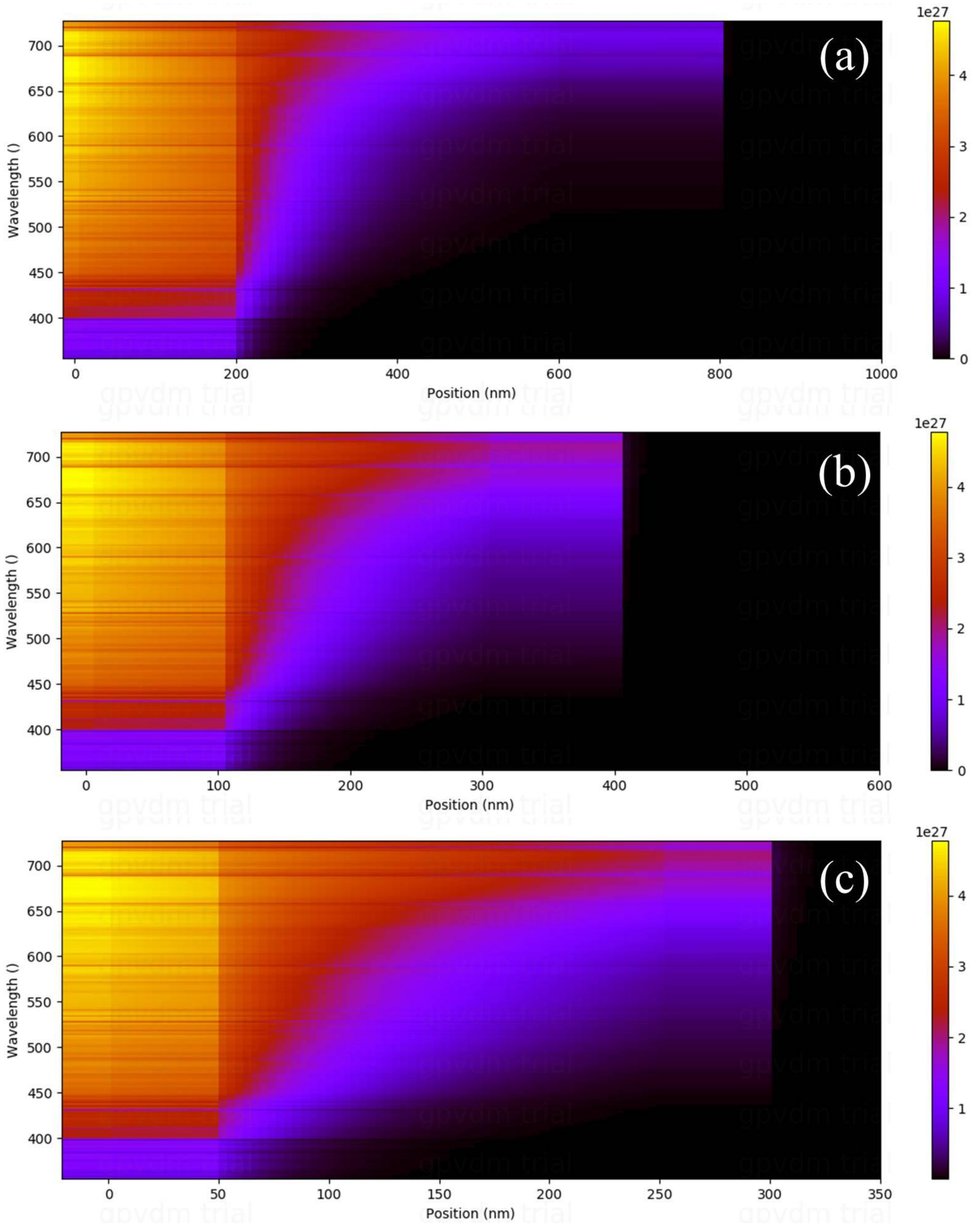

Figure-2 Spectral distribution of incident photons across (a) PSC-1, (b) PSC-2 and (c) PSC-3 configurations

ISSN: 0971-1260
Vol-22-Issue-16-August-2019

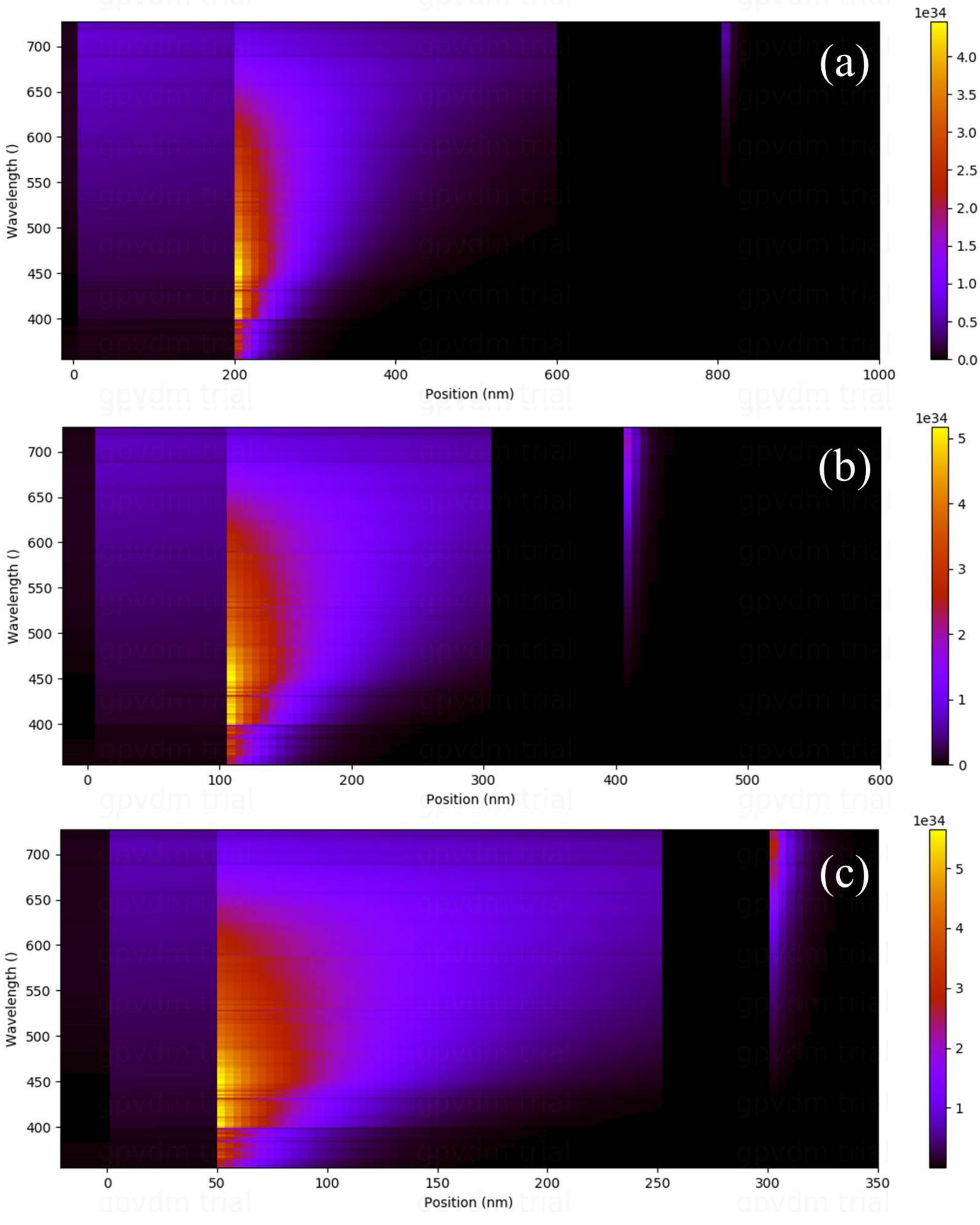

Figure 3 Spectral distribution of absorbed photons across (a) PSC-1, (b) PSC-2 and (c) PSC-3 configurations

ISSN: 0971-1260
Vol-22-Issue-16-August-2019

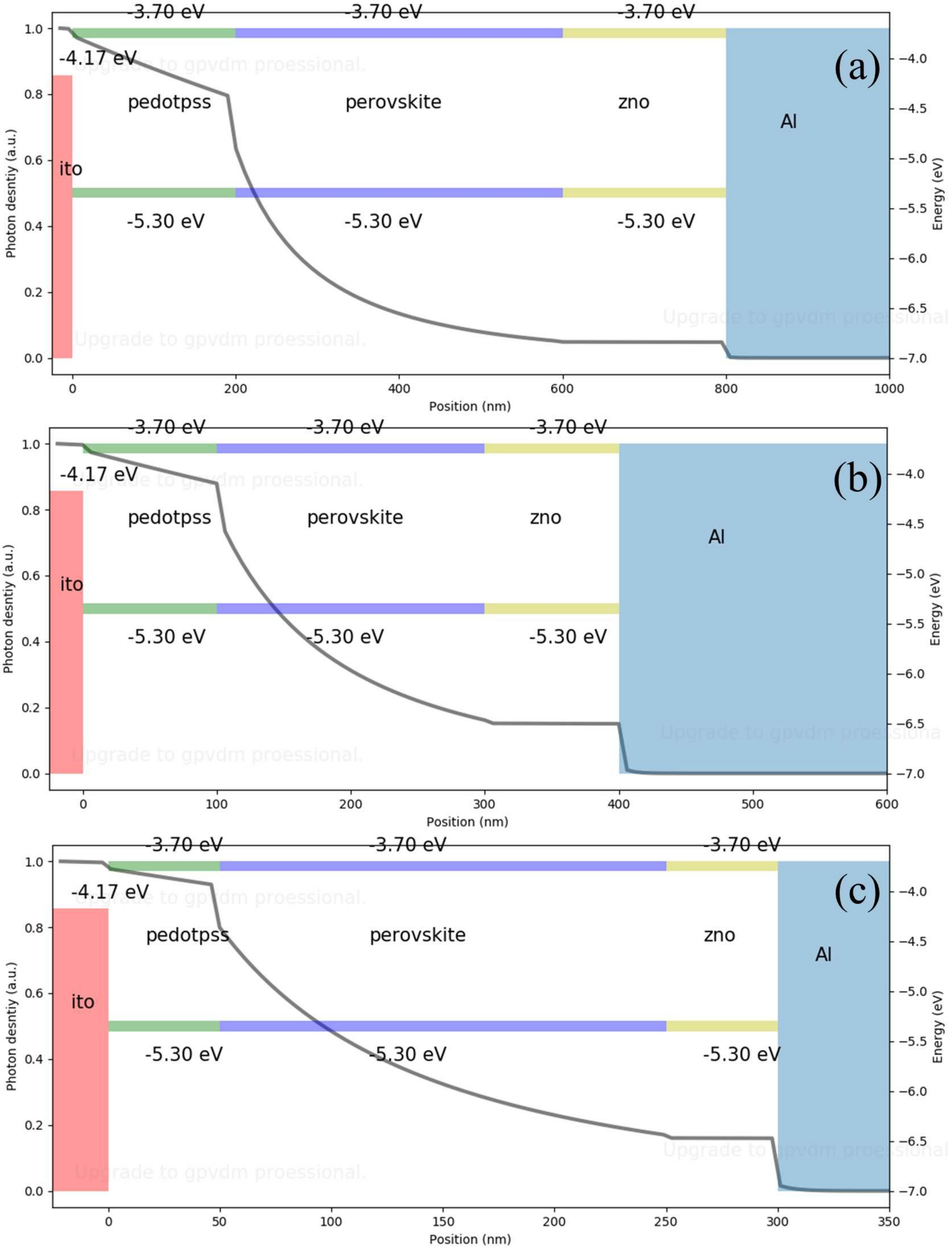

Figure 4 Photon density variation across (a) PSC-1, (b) PSC-2 and (c) PSC-3 configurations

ISSN: 0971-1260
Vol-22-Issue-16-August-2019

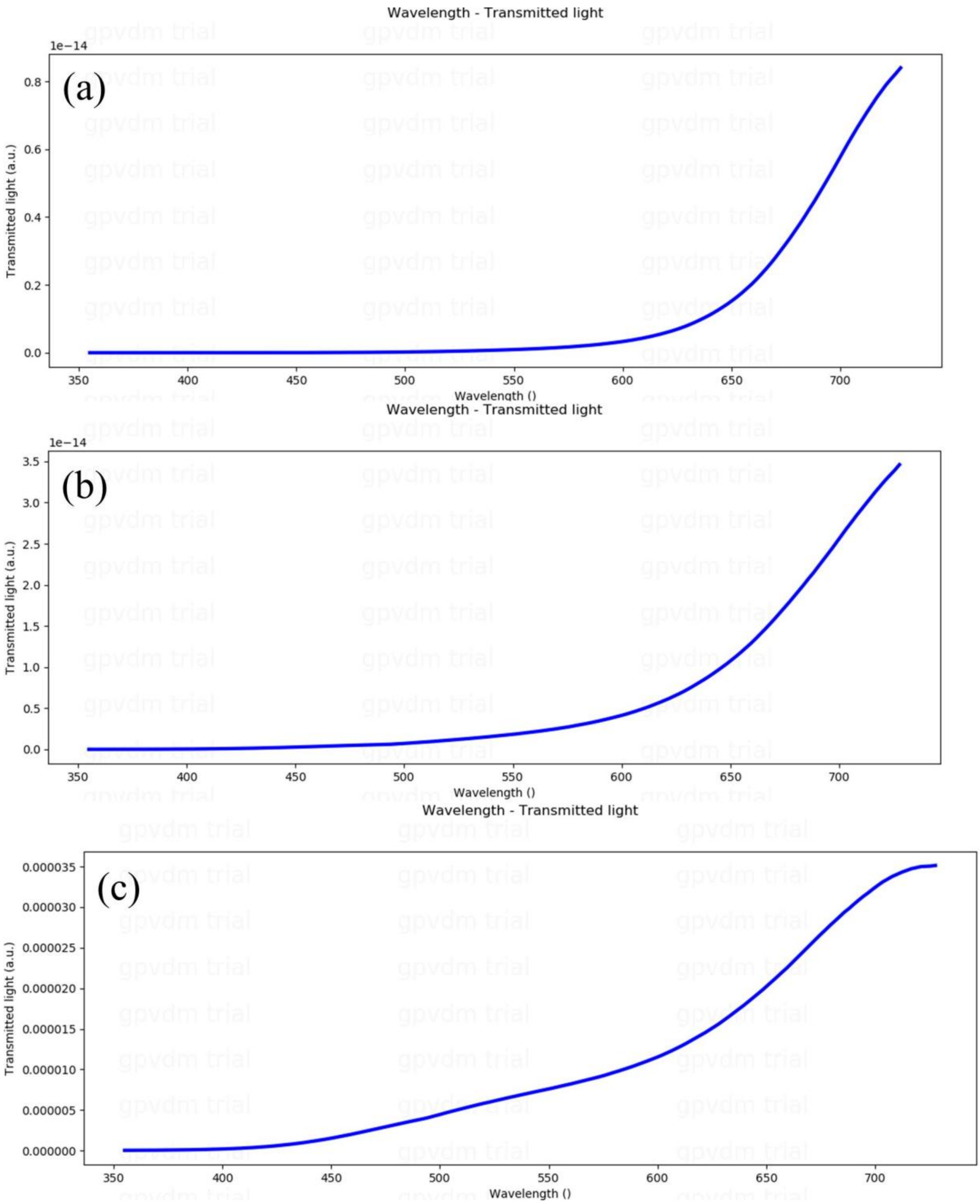

Figure 5 Spectral distribution of transmitted (unutilized) light across (a) PSC-1, (b) PSC-2 and (c) PSC-3 configurations