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Light Trapping for Absorption Control in Perovskite-Based Photovoltaic Solar Cells

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Abstract—Nanostructure based perovskite solar cells with high performance are the focus of study in current work, keeping in view the improvement in cell efficiency. In the first part of the study, a plane-layered solar cell is studied by adding a 1D Photonic Crystal (1D PhC) at the bottom of the cell in order to facilitate the photon rotation process. However, in the second part of the study, it is observed that the addition of grating enhances the light absorption due to photon trapping. Following that, the light absorption of three different structures is compared. The observations reveal that the short-circuit current density (Jsc) is found to be $-39.93\,\mathrm{mA/cm^2}$, which is 87.29% higher than that for a planar structure exhibiting the short-circuit current density (Jsc) value of $-21.32\,\mathrm{mA/cm^2}$. Finally, the efficiencies of these nanostructured perovskite solar cells are found to be significant. For the proposed solar cell structure an 87.24% improvement in the power conversion efficiency (PCE) is observed, i.e., from 14.03% for the planar structure to 26.27%.

1. INTRODUCTION

For widespread use of solar energy, cost-effective photovoltaic (PV) devices exhibiting higher conversion efficiency are expected. The recent introduction of perovskite materials, especially organic-inorganic halides ($CH_3NH_3PbX_3$, X = Cl, Br, I), has opened up new possibilities for low-cost Photovoltaic (PV) modules [1, 2]. The efficiency of perovskite solar cells has been observed to improve from 3.8% to roughly 25% in just a few years of development [3–6]. To improve the efficiency of perovskite-based solar cells, a variety of strategies have been reported so far, including the engineering of interface materials [7, 8], optimization of fabrication processing [6], mesoporous scaffold designs [9], etc. The fundamental goal of these schemes is to improve the electrical characteristics (high conversion efficiency) of solar cells by reducing carrier losses.

The balance between electrical and optical characteristics of perovskite-based solar cells to achieve high performance can be controlled by effective light management. The light losses can be reduced by trapping more photons in the active layers of solar cells.

In a basic perovskite-based solar cell, an active layer ($CH_3NH_3PbI_3$) is placed between the Hole Transport Layer (HTL) and Electron Transport Layer (ETL) [6, 8]. High conversion efficiency would only be possible by improving the collecting efficiency and reducing carrier recombination while configuring a solar cell. Electrical benefits such as increased mobility and carrier life, as well as lower defect density, can only be realized by improving the quality of the perovskite material used as an active thin layer [10]. A thin absorbing layer, on the other hand, cannot provide adequate carries through light absorption. In fact, trapping photons in a thin active layer would be the ultimate solution regarding the

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absorption of maximum incident light. One can conclude that improved optical and electrical properties of perovskite-based solar cells are possible by introducing a nanostructured active layer.

The method is named "photon reusing" [11], in which an ordinary metallic layer of aluminum (Al) or silver (Ag) is utilized as a back reflector and exhibits reflectance greater than 90%. However, a metal-semiconductor interface presents undesirable misfortunes due to the existence of surface plasmons. Moreover, metallic surfaces are destructive in nature due to their restricted diffraction capabilities and high corruption rates [12, 13].

Organic-inorganic halide perovskite materials such as photonic crystals can further improve the efficiency of such cells. Photonic crystals are widely used for light trapping in solar cells due to the alternate arrangements of dielectric material used effectively to control the light as desired; hence they are [6].

Herein, we report the preparation of a hybrid perovskite solar cell with a photonic crystal at the bottom acting as a selective light reflector and helping to reuse the photons within the cell thereby increasing the overall absorption efficiency of a nanostructured perovskite-based solar cell. To validate large-scale production, a 1D photonic crystal was incorporated to keep the device thin. In the proposed structure, the alternate layers have been optimized using RSOFT's Diffract MOD and Solar Cell Utility, based on the Rigorous Coupled Wave Analysis (RCWA). This structure can offer improved retention of photons with a center wavelength of 600 nm.

2. STRUCTURAL OPTIMIZATION

The proposed solar cell structure (Fig. 1) comprises perovskite materials based on organic-inorganic halides ($CH_3NH_3PbX_3$, where X = Cl, Br, and I) with a safeguard layer of ~ 700 nm, a hole transport layer (HTL) of P3HT — poly(3-hexylthiophène), and an effective electron transport layer (ETL) of zinc sulfide (ZnS). The thickness of the **HTL** and **ETL** layers is kept at ~ 20 nm, with a grating of ~ 510 nm for the ZnS layer. The **Zinc Sulfide (ZnS)** can also act as a buffer layer between the **ETL** and photonic crystal. The conductive oxide in the proposed structure was fluorine-doped tin oxide (FTO), which was used as a part of the reflector structure. The trapping of photons was done through diffraction gratings by diffracting the incident light to certain parts of the solar cell with a distinct order of diffraction.

In simulations, the parameters related to grating are fixed as: period of back structure as $\Lambda = 0.72\lambda g$ and grating depth as $t = 0.18\lambda g$, where λg is the energy band gap for silicon with a value of 1.107 µm.

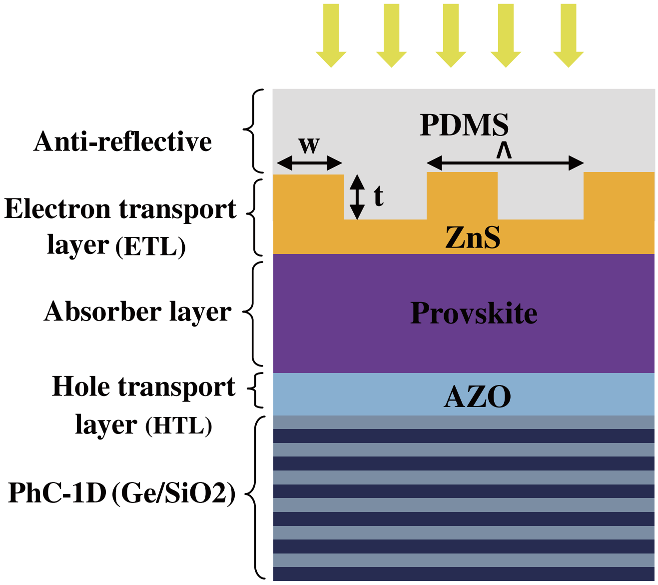


Figure 1. Proposed perovskite-based solar cell structure.

The 1D photonic crystal as part of the back reflector can double the optical path since it is also a critical part of the light-trapping structure due to the reuse of reflected photons. The thickness of a 1D photonic crystal was set to be one-fourth of the overall thickness of the cell. Actually, the 1D photonic crystal is a stack of 7 pairs of Ge/SiO_2 ($n_\mathrm{h}/n_\mathrm{l} = 3.5/1.46$). This ratio is decided by the center wavelength, λd. The impact of the center wavelength is depicted in Fig. 1, which outlines the impact of the 1D PhC. It has been observed that the selection of the center wavelength is more important for thinner cells than the thicker ones. For thicker solar cells, the maximum number of incident photons can be ingested, which ultimately reduces the retention of photons. Moreover, it has also been noticed that the selection of the center wavelength is not vital for a thicker solar cell, as shown in Fig. 1. The observations revealed that the center wavelength λd of 0.60 µm can propose leading execution for solar cells with overall thickness in the range from 5 µm to 20 µm.

3. RESULTS AND DISCUSSION

The behavioral analysis of the proposed solar cell and computation of the power conversion efficiency (PCE) were carried out using RSOFT's Diffract MOD and Solar Cell Utility based on the RCWA calculations. The RCWA calculations give a quick and productive strategy to illuminate Maxwell's conditions. The strategy could be a semi-analytical procedure, which means that it picks one course (longitudinal) to disentangle logically, and the other two (transverse) courses to be measured numerically and productively decide reflection and transmission from the periodic structures. It employs a discrete Fourier change to observe the areas within a transverse heading. This strategy would consider materials and areas as a set of plane waves (or planar gratings). For unaltered plane waves, the RCWA is an amazingly quick and proficient gadget used to record differentiation. However, the longitudinal direction is measured systematically, so layers of any thickness would not influence the computational burden [14–16]. The whole number of approaching photons at occurrence sun-based range $S\left(\lambda\right)$ is given as:

$$n_s\left(\lambda\right) = \frac{S\left(\lambda\right)}{E\left(\lambda\right)} = \frac{\lambda}{hc} S\left(\lambda\right) \tag{1}$$

where $E\left(\lambda\right)$ represents the energy for incident photons. The entirety of assimilation spectra for every layer describes the overall retention range of gadget as:

$$A\left(\lambda\right) = \sum A_i(\lambda) \tag{2}$$

RSoft's CAD tool was used to compute the absorption spectra. The number of photons retained by each layer was described as follows:

$$n_i\left(\lambda\right) = \frac{S\left(\lambda\right) A_i\left(\lambda\right)}{E\left(\lambda\right)} = \frac{\lambda}{hc} S\left(\lambda\right) A_i\left(\lambda\right) \tag{3}$$

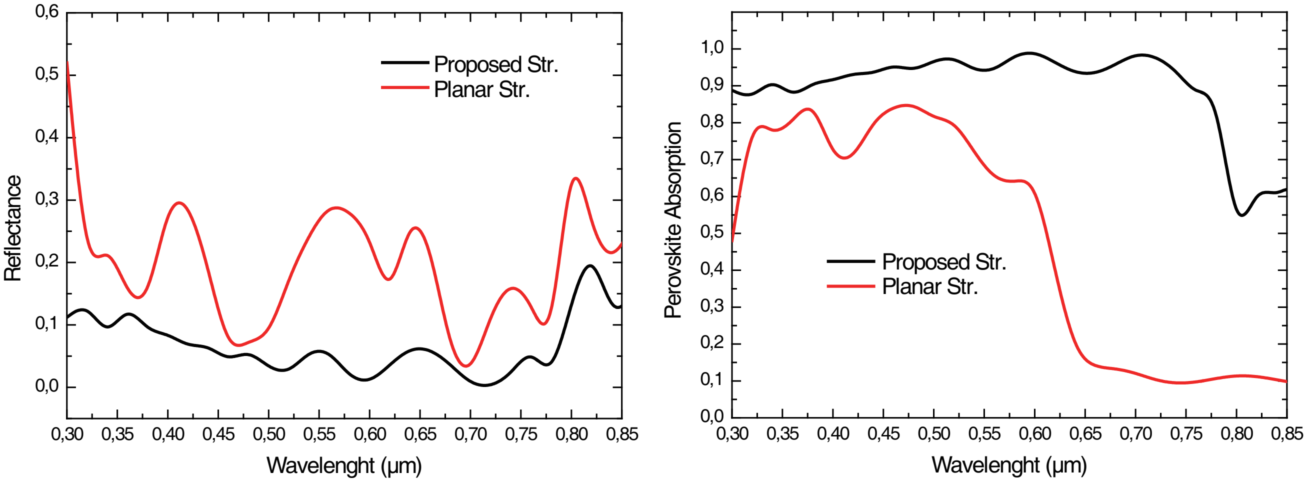
Finally, the overall efficiency of the solar cell was computed as follows:

$$\eta\left(\%\right) = \frac{J_{sc} \cdot V_{oc} \cdot FF}{P_{in}} 100 \tag{4}$$

As the photons are trapped inside the proposed structure, there will be a significant reduction in the reflection of incident light as shown in Fig. 2(a). The trapped photons will ultimately result in an improved profile of the electric field inside the proposed structure of the solar cell as shown in Fig. 2(b). It has been observed that 90% of the incident photons can be retained within the extended thickness of the cell from 300 nm to 800 nm due to a significant reduction in optical parasitic and reflection losses. In this manner, an increment is evident in the integrated spectrum of the proposed structure.

The proposed structure was simulated for a proposed thin film perovskite solar cell with and without grating (Fig. 3).

It has been observed that the results with and without grating are compared within the wavelength range of $\sim$ 300 nm to $\sim$ 1200 nm. The calculations for conversion efficiency and short circuit current for the planar and proposed cell structures reveal that the addition of gratings improves specific cell parameters by increasing light absorption due to photon trapping at the bottom of the cell (Table 1 and Fig. 3).



(a) (b)

Figure 2. (a) Normalized reflectance and (b) absorption spectra, for planar and proposed structures.

Table 1. Comparison of the power conversion efficiency and short circuit current of proposed thin film perovskite solar cell with and without grating.

Device Structure	**PCE%**	**Jsc (mA/cm^2)**
Planar Str.	14.0268%	21.3248 mA/cm^2
Proposed Str.	25.4411%	38.6778 mA/cm^2

In a previous study, we found that the addition of photonic crystal at the bottom of the cell significantly upgraded the retention of incident photons in the solar cell.

One of the major advantages of utilizing dielectric 1D photonic crystal as compared to a metal back reflector and metal semiconductor interface is that photonic crystal offers minimal diffraction losses and surface plasmon reverberation [17, 18].

In this segment, a strategy for optimizing structure is displayed. In solar cell applications, a cell is required to have high control change productivity and great brief circuit current. The observations reveal that the PCE is expanded as the discussed layer is made thicker.

In order to examine this issue, a structure with $(d_{SiO_2}/d_{Ge})_j = 0.2\,\mu\text{m}$ has been considered. The number of intermittent layers within the photonic gems has not been changed and is taken as four. Presently, in the proposed method, only the thickness of the layers within the 1D photonic gems is changed.

Each photonic crystal's layer thickness is changed linearly by a constant value. Fig. 4 depicts a 1D photonic crystal with linearly shifting layer thicknesses. The thickness of the layer in a photonic crystal is increased as,

$$(d_{SiO_2}/d_{Ge})_j = (d_{SiO_2}/d_{Ge})_1 + (j-1)\,(\&B) \quad j = 1, 2, \ldots, n \tag{5}$$

where $(d_{SiO_2}/d_{Ge})_1 = 0.1\,\mu\text{m}$ is the thickness of the first air layer; $(\&B) = 0.03\,\mu\text{m}$ is the amount that is added to the air layer thickness in each step; and $n = 7$ is the number of periodic layers in the photonic crystal.

The thickness of the pair layer in the photonic crystal is decreased as;

$$(d_{SiO_2}/d_{Ge})_j = (d_{SiO_2}/d_{Ge})_1 + (n-j)\,(\&B) \quad j = 1, 2, \ldots, n \tag{6}$$

The values of the varying parameters are the same as before. As a result, the pair layer thickness in the photonic crystal increases linearly from 50 nm to 220 nm and then decreases linearly from 220 nm to 50 nm to achieve a higher PCE of the cell.

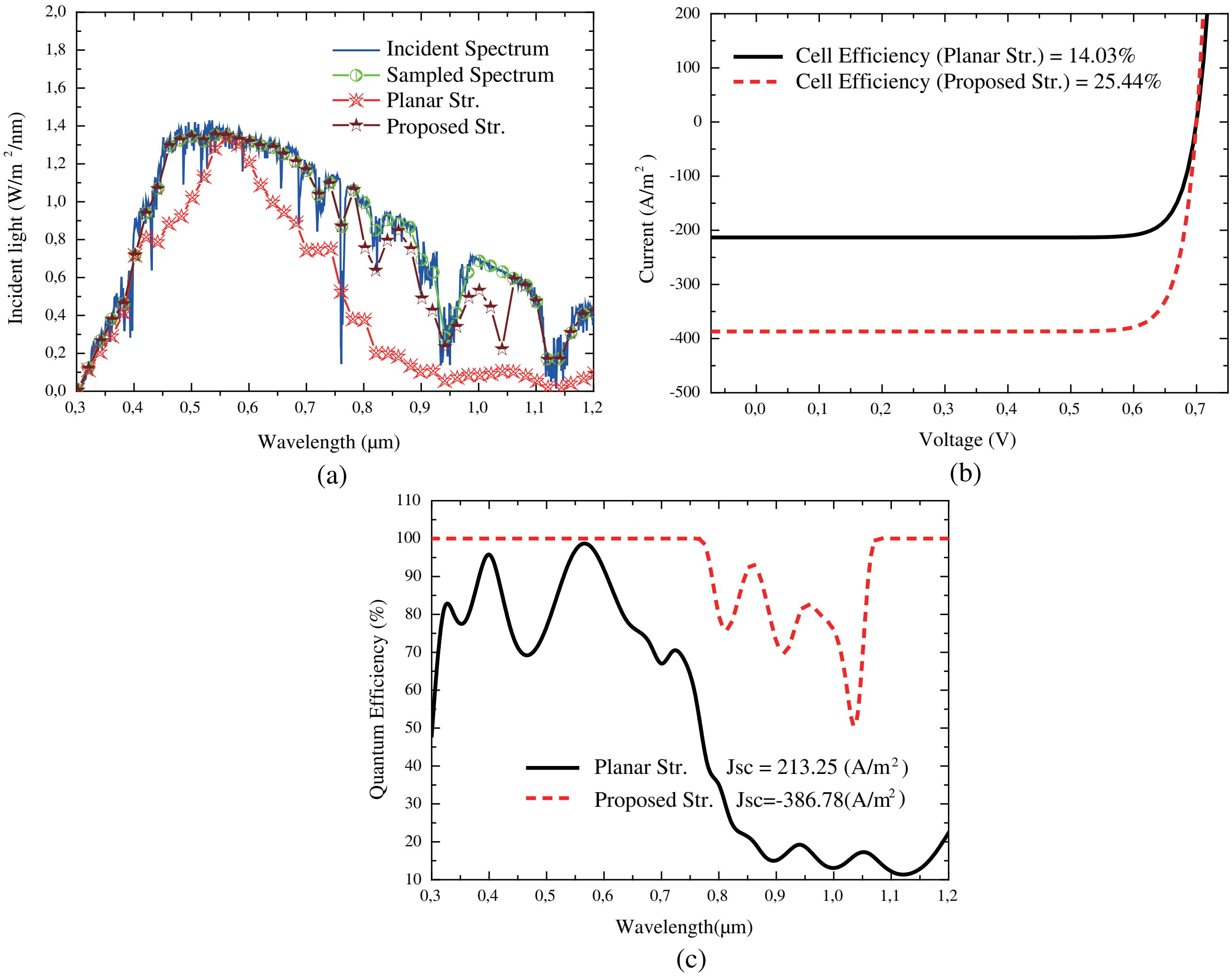


Figure 3. (a) Absorption spectrum, (b) solar cell J-V curve and (c) quantum efficiency Vs wavelength.

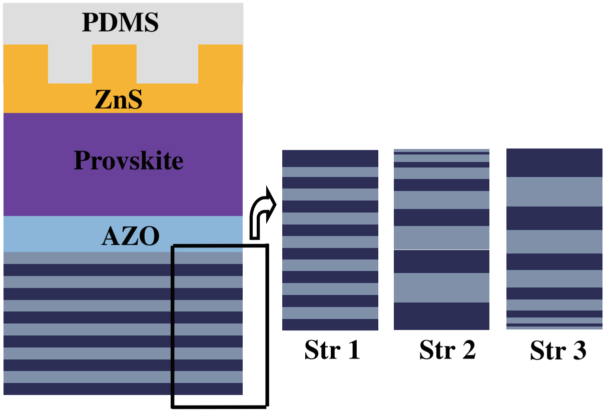
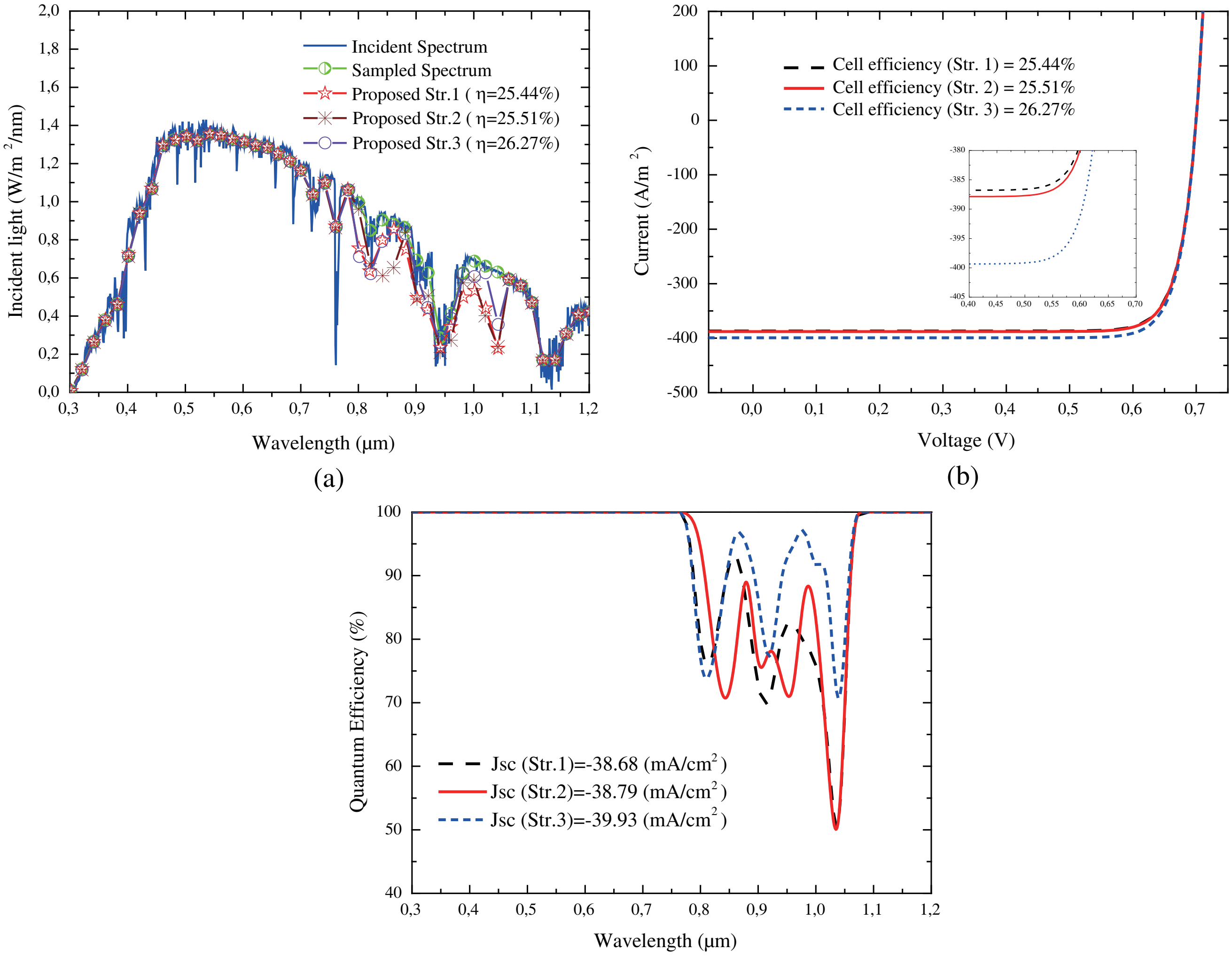


Figure 4. Perovskite-based solar cell with PhC-1D (Ge/SiO_2) with different configurations of layer PhC-1D layers, **(Str 1)** The thickness of layer PhC-1D is equal, **(Str 1)** The thickness of layer PhC-1D is from smallest to largest, **(Str 1)** The thickness of layer PhC-1D is from largest to smallest.



(a) (b)

(c)

Figure 5. (a) absorption spectrum, (b) solar cell J-V curve, (c) quantum Efficiency Vs wavelength, for the three structures.

In this case, after using such a thick layer, the structure would be nearly level. Fig. 1 shows that three distinctive assumptions approximately create the cell. In each hypothesis, the primary structure of the photonic crystal was optimized to investigate the impacts of three structures on cell performance. Fig. 5 shows the absorption of incident solar spectra, J-V curve, and quantum efficiency vs. wavelength. The absorption spectra reveal only a few changes in the range from 750 **nm** to 1000 nm (Fig. 5(a)). The highenergy incident photons can be absorbed by the upper portion of the photonic crystal and exhibit no significant interactions within the lower layers of the perovskite.

Figure 5(b) depicts the characteristics of the current profile in terms of voltage for all three proposed structures. As anticipated, the reduced reflection and parasitic losses in addition to the enhanced absorption of light within the perovskite layer due to trapping resulted in an improved Jsc for the proposed structure as compared to that for a planar PSC.

As shown in Table 2, the Jsc for structure 3 is $-39.93\,\mathrm{mA/cm^2}$, which is expanded by 2.96% as compared to structure 2 and 3.23% to structure 1. The Voc has also been increased and now stands at 0.78 volts.

The transformation proficiency is additionally expanded by 3.26%, from 25.44% the structure 1 to 26.27% the structure 3.

Table 3 reports the state of the power conversion efficiency for different perovskite solar cell

Table 2. Comparison between the PCE and the Jsc for different proposed structures.

Device Structure	**PCE%**	**Jsc ($\mathbf{mA/cm^2}$)**
Str. 1	25.4411%	$-38.6778\,\mathrm{mA/cm^2}$
Str. 2	25.5126%	$-38.7865\,\mathrm{mA/cm^2}$
Str. 3	26.2676%	$-39.9343\,\mathrm{mA/cm^2}$

Table 3. Comparison of the power conversion efficiency for different solar cell structures based on perovskite materials.

References	**back reflector**	**PCE%**
[22] [2020]	Semitransparent	14.96
[19] [2016]	Silver nanoparticles	16.04
[20] [2018]	Gold nanoparticles	15.94
[21] [2020]	metallic layer of gold	24.93
[23] [2018]	1D photonic crystal	25.44
This work	Proposed structure	26.27

structures [19–23]. We can conclude that the proposed solar cell structures exhibit a good performance compared to other devices.

4. CONCLUSIONS

In summary, coupled optical-electrical simulations were carried out to investigate the optical and electrical properties of PSCs. Firstly, the light losses in a planar architecture have been investigated, and a nanostructure-based solar cell on a textured silicon substrate was proposed to mitigate these losses. The observations revealed that the use of PDMS instead of glass in the suggested structure decreases the overall reflection losses. Moreover, the light trapping phenomenon in the active layer would result in enhanced absorption and SPR far-field scattering. The effect of reduced thickness for the HTL on the optical characteristics of the cell has also been investigated. The absorption of perovskite in the proposed structures was found to be similar to that of the main structure, and the PSCs exhibit considerable efficiency. The current-voltage characteristics revealed improvements in Jsc and Voc. The PSC's power conversion efficiency was observed to increase from 14.03% to 26.27%. The simulation data describes that the PCE of 90% compared to the planar structure is the evidence for a significant efficiency boost.

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