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Efficiency Enhancement in Dye Sensitized Solar Cell Using 1D Photonic Crystal

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Abstract

1D SiO_2/TiO_2 photonic crystal based ZnO-Pt DSSC with N719 dye is theoretically designed. The optical properties of theoretically designed DSSC such as transmittivity, Absorptivity and reflectivity are calculated using transfer matrix method in order to calculate numerically the key parameters like open circuit voltage (V_{OC}), Photo current density (J_{ph}) of the DSSC. It is found that the desired integrated system may enable to maximize the absorption in the selective spectrum region (400-900nm) and hence the maximum efficiency achieved is 4.5 % for a 1D SiO_2/TiO_2 photonic crystal layers with two number of periods.

Key words: Photonic crystal, Absorber, Dye sensitized solar cell, Efficiency.

Introduction

Dye-sensitized solar cells (DSSCs) have emerging as a technical and economical sustainable substitute to the p-n junction photovoltaic devices. The chlorophyll-form sensitized zinc oxide electrode based DSSC was synthesized in 1972 [1]. Recently sensitized solar cells like DSSCs and quantum dot sensitized solar cells (QDSCs) are promising low-cost option to conventional photovoltaic devices based on materials such as Si and CdTe due to their lower cost and effortless fabrication process [2-3]. A Number of research has been executed on ZnO single crystals, even so the efficiency of these dye-sensitized solar cells were very down and out being as the monolayer of dye molecules was capable to absorb incident light intensity only around 1% [2]. Thus, optimizing the porosity of the electrode made up of refine oxide powder upgrade the efficiency of DSSC. Hence the dye absorption over electrode might be enhanced to improve the light harvesting efficiency (LHE).

Nano porous titanium dioxide DSSC with 7% efficiency were discovered in 1991[3]. Although various studies have been reported that the absolute efficiency of TiO_2 DSSCs is always higher than that of ZnO DSSCs efficiency [4]. This is because of the presence of the high carboxylic acid essential groups in the dyes in which the dissolution of ZnO and precipitation of dye-Zn^{2+} complexes occurs. This occurrence results in a deficient overall electron injection efficiency of the dye.

The overall power conversion efficiency have been focused on increase the photovoltage through function of the oxide, improving the photocurrent with new dyes, and boosting stability by better encapsulation [5]. By the use of liquid electrolyte in DSSCs in the spectral range around 520 nm.

Intense research efforts largely focused on synthesizing new organic dye molecules with higher absorptivity materials as were invented more efficient carrier transport layers [6]. The photon management conception has presently plays an important research field to enhance LHE in photovoltaics. Several theoretical approaches are reported already on a variety of possible effects including the localization of heavy photons near the edges of a photonic bandgap [7], Bragg diffraction in a periodic lattice [8], multiple scattering at disordered regions in the photonic crystal (PhC) [9], and the formation of multiple resonant modes [10]. One approach to strongly strengthen the LHE is using optical elements, such as highly scattering layers. This consist of Photonic Crystal (PhC) absorption layer with ZnO photo anode on DSSC that increases the photon path length in the cell [10-12].

Nanostructured materials, such as PhCs, large particle aggregation scattering layers, and plasmonic nanometals have opened to increase LHE in the third-generation solar cells [13-16]. PhCs, with periodic dielectric nanostructures, view strong ability to attain a unique level of control the light propagation are also light energy distribution in photovoltaic devices [17-19]. In these devices via several mechanisms, such as photon localization increase the red light absorption near the red edge of a photonic bandgap, light reflection within the photonic bandgap at various angles and formation of photon resonance modes within the solar cell are used to increase the LHE [16,17]. Hence photovoltaic devices integrated with PhCs, photons absorption increases which results increased LHE with lower usage of absorbing materials. The first verification of light absorption enhancement outcome of PhC coupled sensitized solar cells in 2003 has stimulated more and more efforts to design PhCs with different optical structural and properties that permit for light management in the cells [20].

In this work it is plan to investigate on theoretical design of porous nature of Zno-Pt DSSC with N719 dye. Optical properties of theoretical designed DSSCs such as transmittance, reflectance and absorptance are calculated using Transfer Matrix Method (TMM), in order to calculate numerically, the key parameters like open circuit voltage (V_{oc}), Photo current density (J_{ph}), efficiency etc. In addition, the efficiency of porous 1D SiO_2/TiO_2 PhC coupled ZnO-Pt DSSC is calculated and compared with Zno-DSSC without PhC.It is concluded that the presence of porous 1D SiO_2/TiO_2 PhC enhance the efficiency of DSSC.

Construction of DSSC

The DSSC structure comprised by FTO, ZnO photoelectrode, N719 dye, KI electrolyte solution with platinum counter electrode was theoretical designed. Probably, DSSCs are usually built with two layers of conductive transparent media that allow a medium to deposit the semiconductor and catalyst. Here the porous ZnO nano-particle semiconductor film is deposited on transparent conducting oxide (TCO)-coated glass substrate which act as a photo electrode and Platinum deposited TCO serves as a counter electrode respectively [21]. The N719 dye is the component of DSSC responsible for the maximum absorption. It is anchored to the ZnO nano-particle surface with liquid KI electrolyte. Redox couple should be able to regenerate the oxidized dye efficiently.Both operating ZnO and Pt counter electrodes are bound together, and an electrolyte KI is then loaded with aid of a syringe. Counter electrode catalyzes the reduction of I^{-}/I^{-3} liquid electrolyte and gathers holes from the hole transport material. The figure 1 shows the schematic structure of ZnO-Pt DSSC.

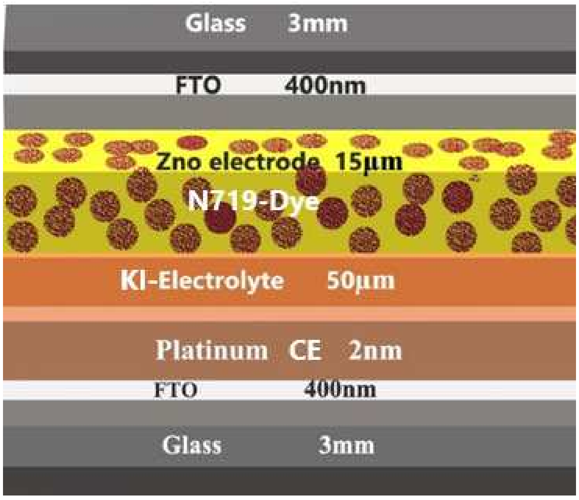

Fig.1.Schematic Structure of the designed DSSC

Optical Properties of ZnO working electrode

The optical properties of the N719 loaded ZnO working electrode are essential to evaluate the absorption of the entire structure of the ZnO DSSC with and without 1D PhC. From the recent literature of experimental research, the estimated absorbance values of the N719 loaded ZnO working electrode is found to be 34.28% for a wavelength of 534 nm having the electrode thickness of 330 nm [22].

The refractive index of N719 loaded ZnO working electrode is calculated from the following equation [24].

$$n = \frac{1 + R + \sqrt{R}}{1 - R} \qquad (1)$$

The calculated refractive index of N719 loaded ZnO working electrode is comparable with various experimental work [25].

The reflectance is calculated from the following equation

$$R = 1 - (A + T) \qquad (2)$$

The transmission of Dyed ZnO is calculated from the absorbance using Beer's lambert law [23].

Table:1. Refractive index and thickness of different layers of ZnO-Pt DSSC device with 1D PhC coupled layer for the wavelength range (400-900nm) [22].

Layers	**Components**	**Refractive index**	**Thickness**
1	Substrate(glass)	1.5	3mm
2	FTO	1.81	400nm(400-600nm)
3	Dyed ZnO	1.94	15μm
4	Dye/SiO_2/KI	1.43	95nm
5	Dye/TiO_2/KI	1.81	88nm
6	Electrolyte	1.42	50 μm
7	Platinum	2.32	2nm
8	FTO	1.81	400nm
9	Substrate(glass)	1.5	3mm

DSSC consists of multiple thin layers with distinct optical properties. The conventional optical TMM is used in this work to calculate the distribution of light intensity in DSSC [25]. A classical interaction exists between the electromagnetic radiation and a finite one-dimensional non-periodic multilayer, where the corresponding Maxwell's equations are solved using TMM formalism. This interaction system fulfils the same conditions proposed by the reflection, transmission and absorption, within the layers, and optical interference between incoming and outgoing optical electric fields [26].

The index of refraction which may be expressed as $n_j(\lambda)=n_j(\lambda)+ik_j(\lambda) = n_j(\lambda)+i\,\lambda\alpha_j(\lambda)/4\pi$ and thickness dj for each layer j. Here nj is the real refractive index, k_j is the imaginary refractive index, and α_j is the absorption coefficient j=1, 2...m, the figure 1 shows the theoretically designed DSSC with actual parameters of different layers. Light of intensity I_0 is assumed to be incident normal to the substrate for a centre wave length of 550nm(λ_0) and multiple reflections at the air/substrate and substrate/ multilayer interfaces are taken into account for the study of transmission spectra of DSSC [27].

Integration of 1D Photonic crystal in DSSC

By employing multilayers made of photonic crystal with multilayers having different lattice parameters is fabricated that possible to increase the photogenerated current for the whole spectral region in which the dye absorbs. Hence the presence of photonic crystal inside the ZnO-Pt DSSC enhance the light harvesting efficiency. In this section, we numerically analyse the integrate system of the ZnO-Pt DSSC with 1D porous SiO_2/TiO_2 photonic crystals shown in figure 2. Initially the optical properties of ZnO-Pt DSSC structure are analyzed using TMM method. Secondly the optical properties of 1D porous SiO_2/TiO_2 photonic crystals coupled ZnO-Pt DSSC are calculated. The PhC structure consist of alternative porous SiO_2 and TiO_2 dielectric layers, whose optical parameters are taken from the literature [28,29]. The thickness of SiO_2/TiO_2 layers are taken as d_{Sio2}=95nm and d_{Tio2}=80nm. The figure (2) shows that the porous 1D SiO_2/TiO_2 PhC coupled DSSC.

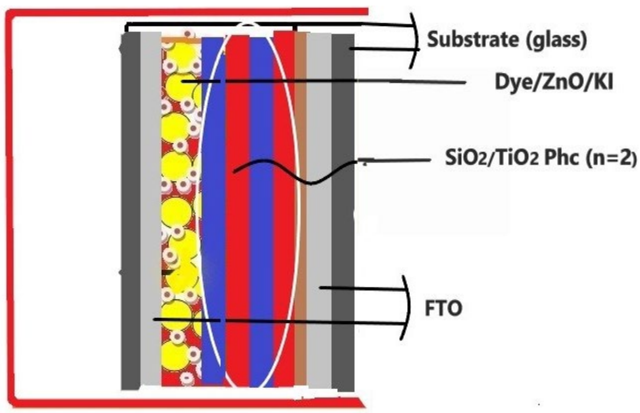

Fig.2.Schematic Structure of the 1D SiO_2/TiO_2 PhC coupled DSSC

The matrices are formed for the intersection between two layers and wave propagation through each layer. The product of all the transfer matrices forms the actual transfer-matrix of solar cell. The photon absorption of these two solar cell designs (with and without PhC) has been favorably compared with the state-of-art solar cell designs. The combination of sub cell layers has yielded very high photon absorption through the entire solar radiation spectrum. The layers can represent in a matrix form in which the product of the individual layers are matrices [7]. Finally, this method involves the system converting the matrix into reflection, transmission and absorption coefficient [31].

According to TMM, each single layer has a transfer matrix the M is given by [7-8].

$$M = \begin{bmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{bmatrix} = \begin{bmatrix} \cos\delta & \frac{i}{\gamma_l}\sin\delta \\ i\gamma_1 \sin\delta & \cos\delta \end{bmatrix} \quad (3)$$

The phase difference is $\delta = \left(\frac{2\pi}{\lambda_0}\right) \times \gamma \times t \times \cos\,(\theta)$

$\lambda_0 - Centre\ \ wavelength,\quad t - Thickness\ \ of\ \ incident\ \ layer,\quad \gamma - refractive\ index\ of\ \ layer$

The product of each intermediate layer starting with air layer, the resulting products describes entire stack in the order in which lights encounter them. Since each layer associated with its own transfer matrix, for our theoretically designed photonic crystal based DSSC system, the matrix describing the number of layers between the air and substrate according to Macleod et.al is given by

$$M_{total} = M_1 * M_2 * M_3 * M_4 * \mathrm{M}_5 * (\mathrm{M}_\mathrm{H} * \mathrm{M}_\mathrm{L})^N * \mathrm{M}_6 * \mathrm{M}_7 * \mathrm{M}_8 \quad (4)$$

M_1, M_2, M_3, M_4, M_5, M_6, M_7, M_8 are glass substrate, FTO, ZnO, Dye, electrolyte, platinum, FTO and glass substrate respectively.

M_H and M_L are the corresponding components of the porous SiO_2 / TiO_2 photonic crystal and N is the period of photonic crystal.

$$(M_H M_L)^N = \left(\begin{bmatrix} \cos\delta_H & \frac{i}{\gamma_H}\sin\delta_H \\ i\gamma_H \sin\delta_H & \cos\delta_H \end{bmatrix} \times \begin{bmatrix} \cos\delta_L & \frac{i}{\gamma_L}\sin\delta_L \\ i\,\gamma_L \sin\delta_L & \cos\delta_L \end{bmatrix} \right)^N \quad (5)$$

For the entire structure of photonic crystal based DSSC, the total transfer matrix is given by

$$M_{total} = \begin{bmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{bmatrix} \quad (6)$$

where the matrix elements can be achieved in terms of the elements of the single-period matrix.

From the total matrix, the transmission coefficient,transmittivity T, reflection coefficient ρ, reflectivity R and absorptivity A can be found. To define R, T, and A, the reflection coefficient is

$$\rho = \frac{\gamma_0 m_{11} + \gamma_0 \gamma_s m_{12} - m_{21} - \gamma_s m_{22}}{\gamma_0 m_{11} + \gamma_0 \gamma_s m_{12} + m_{21} + \gamma_s m_{22}} \quad (7)$$

The reflectivity is $R = \rho \times \rho^*$ (8)

Where the asterisk denotes the complex conjugate

The reflection coefficiencts is

$$\tau = \frac{2\gamma_0}{\gamma_0 m_{11} + \gamma_0 \gamma_s m_{12} + m_{21} + \gamma_s m_{22}} \qquad (9)$$

The transmittivity is $$\mathrm{T} = \mathrm{Re}\left(\frac{\eta_L}{\eta_1}\right)\tau\tau^* \qquad (10)$$

The Absorptivity is calculated from A=1-(R+T) (11)

The Absorptivity is

$$A = \frac{4\gamma_0 (m_{11} + m_{12}\gamma_s)(m_{21} + m_{22}\gamma_s) - \gamma_s}{\gamma_0 m_{11} + \gamma_0 \gamma_s m_{12} + m_{21} + \gamma_s m_{22}} \qquad (12)$$

Where γ_0, γ_1 – Re*fractive indices of air(first) and substrate(last) layer of the DSSC structure*

Calculated photovoltaic properties of 1D SiO_2/TiO_2 PhC coupled ZnO-Pt DSSC

In this work the photocurrent density(J_{ph}), voltage(V_{oc}), saturation current(J_0),quantum efficiency and also power conversion efficiency of ZnO-Pt DSSC are theoretically calculated. and compared with corresponding numerical calculation carry out through1D Sio_2/Tio_2 PhC coupled ZnO-Pt DSSC beside the platinum counter electrode.

The photocurrent density is calculated from the following equation [33].

$$J_{ph} = e \int_{\lambda_{\min}}^{\lambda_{\max}} A^* \phi_T(\lambda)\, \mathrm{d}\lambda \qquad (13)$$

$where\ e - electron\ charge, A -\ Total\ absorbtion\ of\ Zno - Pt\ DSSC\ calculated\ from$ [24]

$$\varphi_T = \frac{p_{in}}{w_{ph}} = \frac{1000}{509 \times 10^{-21}} = 1.96 \times 10^{21} m^{-2} s^{-1}$$

$w_{ph} = h^* f_g\ \&\ p_{in} - incident\ flux\ at\ solar\ spectrum\ A.M\ 1.5\ is\ 1000\ W/m^2$

$$f_g = qW_g / h$$

$where\ W_g\ is\ the\ bandgap\ of\ ZnO\ is 3.37 eV$

$$V_{OC} = \frac{KT}{e}\ln(\frac{J_{ph}}{J_0}+1) \qquad (14)$$

J_{ph} *calculated from equation* (10)

$$J_0 = -2e\pi\int_0^{\lambda_g}\frac{2\,hc^2}{\lambda^5}[\exp(\frac{hc}{\lambda K_B\,T})-1]^{-1}\,d\lambda \qquad (15)$$

$$h = \text{planck's constant}, \quad c = \textit{velocity of light}, \quad [\exp(\frac{hc}{\lambda K_B\,T})-1] \approx -1$$

The fill factor may be calculated [31] using the equation

$$FF = \frac{v_{oc} - \ln(v_{oc}+0.72)}{v_{oc}+1} \qquad (16)$$

$$\textit{where } v_{oc} = {eV_{oc}}/{kT}$$

The efficiencies of the theoretical designed DSSC with and without PhC may be calculated using the equation

$$\eta = \frac{J_{ph} * V_{oc} * FF}{P_{in}} \qquad (17)$$

Results and Discussions

The optical parameters such as transmittance, absorptance and reflectance of the DSSC with and without PhC can be calculated using TMM method, by solving the equations (7) to (12) with MATLAB software. The values are calculated and tabulated in the given table 2

Table .2. Transmittivity (T), Absorptivity (A) and Reflectivity (R) measurement of ZnO-Pt DSSC coupled with and without 1D SiO_2/TiO_2 PhC

Wavelength (nm)	ZnO-Pt DSSC								
	without PhC		n=2 (SiO_2/TiO_2)				n=3 (SiO_2/TiO_2)		
	T	A	R	T	A	R	T	A	R
300	0.94	0.02	0.04	0.94	0.04	0.02	0.9	0.04	0.06
400	0.77	0.0038	0.23	0.8	0.04	0.17	0.94	0.01	0.04
500	0.94	0.01	0.17	0.65	0.02	0.33	0.45	0.01	0.54
600	0.93	0.02	0.05	0.52	0.01	0.47	0.35	0.01	0.64
700	0.92	0.02	0.07	0.45	0.07	0.48	0.39	0.03	0.58
800	0.85	0.02	0.13	0.84	0.01	0.15	0.89	0.02	0.1
900	0.63	0.01	0.36	0.82	0.02	0.16	0.88	0.06	0.06

Table 2 indicates that the transmittance, absorptance and reflectance with the different periods (n=0,2,3) of 1D SiO_2 / TiO_2 PhC coupled ZnO-Pt DSSC configuration. Figure 3 shows the optical characteristics of ZnO-Pt DSSC with 1D SiO_2 / TiO_2 PhC coupled layers(n=0,2,3). The effect is more pronounced in the range of 500nm-800nm. In table 1 the Absorptivity result indicates that the photo electrode does not consume incident light in a single pass owing to the low light scattering of the multilayer non-periodic structure. But the presence of 1D SiO_2/TiO_2 PhC coupled inside near the working electrode can be form the scttering centres and strengthen the scattering process by its periodic structure. Light scattering is employed in dye-sensitized solar cells to improve the optical absorption of the incident light [32].

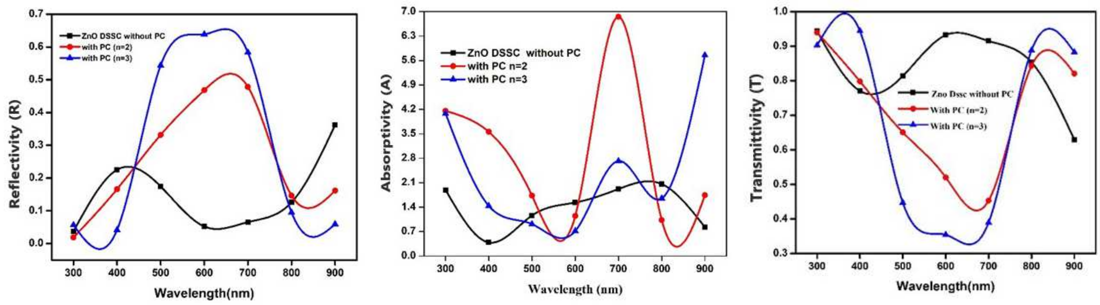

Figure. 3 The reflectance, absorptance and transmittance profile of ZnO-Pt DSSC coupled with and without 1D SiO_2/TiO_2 PhC

From the absorbtion graph it is understood that more absorbtion takes place when DSSC is coupled with PhC. It gets maximum absorption of light inDSSC with PhC having period n=2 compared with PhC having period n=2.It may due to the refractive index contrast make a disorder in the interface of PhC layers. The optimized periods of layers can increase the path length as well as diffused or multiple scattered/reflected and localized the incident light at longer time. As a result, significant optical absorption amplification in a broad spectral range occurs in structures that combine the presence of a 1D photonic crystal and a multi-layer of non-periodically structured absorbing material.

The Photo current density, open circuit voltage for 1D SiO_2/TiO_2 PhC integrated ZnO-Pt DSSC are analysed using equation (13)&(14). The effect is maximum when the DSSC coupled with 1D PhC with period n=2.The effect of Photo current density with number of period of PhC layers is studied and is shown in the figure (4).The short-circuit current increases with the number of period with two.

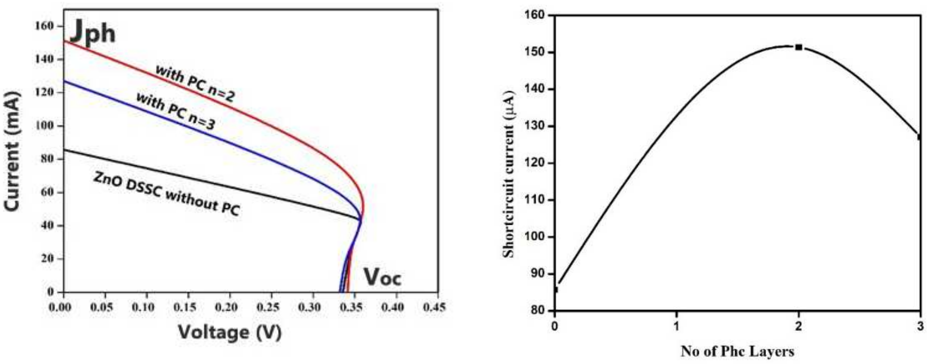

Figure.4. I-V curve and Photo current -vs number of periods of ZnO-Pt DSSC coupled with and without 1D SiO_2/TiO_2 PhC

Because of the increase of optical absorption by multiple reflection / scattering in the interface of PhC structure, it can localize the maximum number of photons on the electrode therefore the short-circuit current is increased in the DSSC. The 1D PhC act as absorber or bottom reflector can trap the incident light. It reduces the group velocity of the photons which can prevent recombination of the excitons for a longer time, hence it leads to the higher rate of photoelectron generation. The lowering of short-circuit current after n=2 is due to the maximum reflection in the forbidden bandgap of PhC. By analysing all the optical parameters and substituted in equation (26), the efficiency of DSSC may be investigated. The calculated J_{sc}, V_{oc}, FF and η for different number of periods in the PhC are shown in the table 3. It is concluded that the DSSC having PhC with period of n=2 get a maximum value of 4.5%.

Table. 3 photovoltaic parameters of ZnO-Pt DSSC coupled with and without 1D SiO_2/TiO_2 PhC

ZnO-Pt DSSC	Number of periods (n)	Jsc(μA cm^{-2})	Voc(V)	FF	ή(%)
SiO_2/TiO_2 (PhC)	0	85.71	0.37	0.75	2.3
	2	152	0.39	0.72	4.5
	3	127	0.38	0.76	3.7

The theoretical results revealed the porous 1D SiO_2/TiO_2 PhC absorbing layer and act as a potential couple layer to improve the efficiency by trapped and initiate the photons drive gradually back through the absorbing electrode in the selective spectrum range 400nm -900nm.

Conclusion

The photovoltaic parameters of ZnO-Pt with N719 dye based DSSC are calculated and also ZnO-Pt coupled with porous 1D SiO_2/TiO_2 PhC with different periods is theoretically designed and analyzed. The absorptance. of the integrated system of ZnO-Pt DSSC with and without 1D SiO_2/TiO_2 PhC are calculated using TMM method. It is found that the desired integrated system may enable to maximize the absorption in the selective spectrum region (400-900nm). The short circuit current (J_{sc}), open circuit Voltage (V_{oc}), Fill factor (FF) and hence the efficiency(ή), are calculated theoretically. The maximum short circuit current (J_{sc}) is found to be 440 $\mu A\ cm^{-2}$ and hence the maximum efficiency achieved is 4.5 %. for a 1D SiO_2/TiO_2 PhC with two number of periods. The optical design of 1D SiO_2/TiO_2 PhC absorbing layer enhance the cell efficiency without affecting kinetic balance between charge separation and recombination.

CONFLICT OF INTEREST

The authors declare that they do not have a conflict of interest

FUNDING

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Author contributions:

There are variety of methods available to increase the efficiency of DSSC. The propagation of light inside the DSSC can be controlled or modulated by the photonic crystals. Hence the photonic crystal embedded solar cell may be used to trap the light and hence to increase the efficiency of the solar cell.

The problem being addressed:

1D SiO_2/TiO_2 photonic crystal based ZnO-Pt DSSC with N719 dye is theoretically designed.The optical properties of theoretically designed DSSC such as transmittance, absorptance and reflectance are calculated. The use of 1D SiO_2/TiO_2 photonic crystal light trapping structures in DSSCs demonstrates the ability to increase the performance of solar to electrical conversion.

Compliance with ethical standards

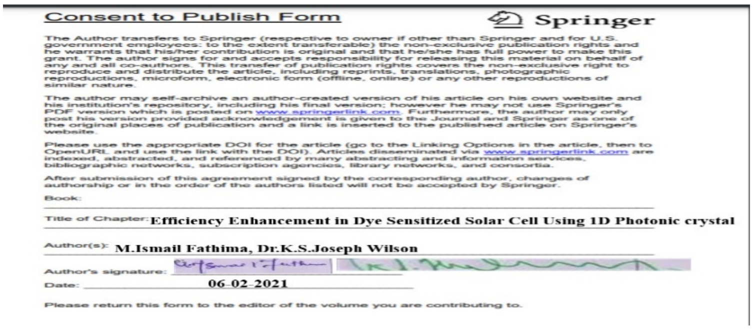
The submitted work should be original and should not have been published elsewhere in any form.

Availability of data and material

The [data type "Photonic structure parameters"] data that support the findings of this study are availablein[**http://www.tandfonline.com/loi/tmop20,**"][**https://www.researchgate.net/publication/334045078**].

Consent to participate : Not Applicable

Consent for Publication



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Figures

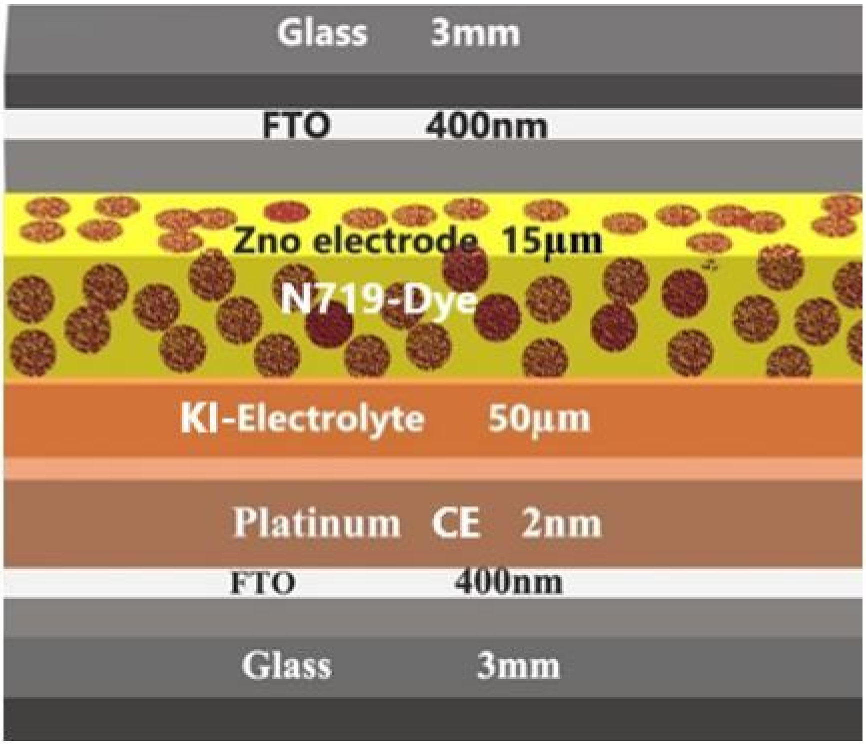

Figure 1

Schematic Structure of the designed DSSC

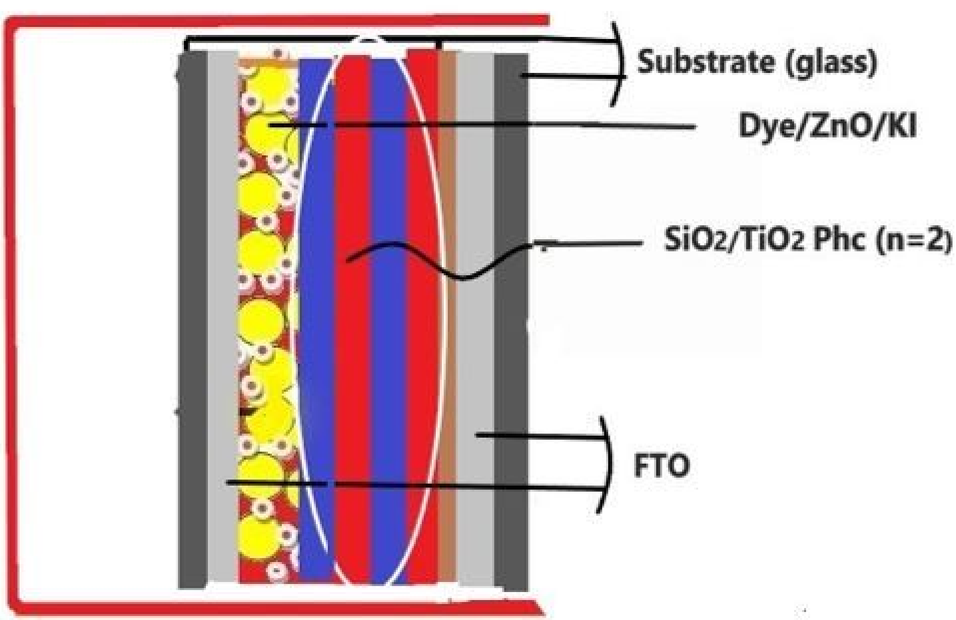

Figure 2

Schematic Structure of the 1D SiO2/TiO2 PhC coupled DSSC

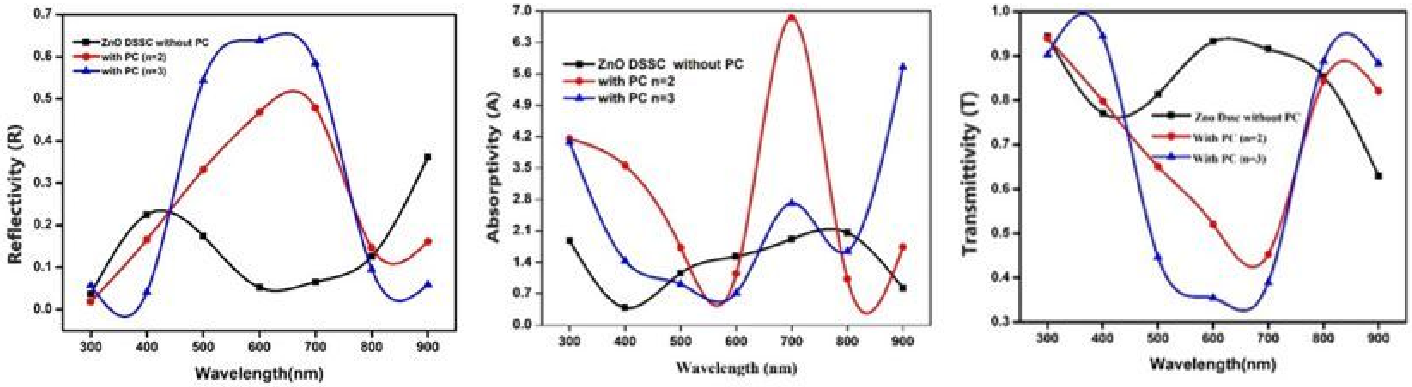

Figure 3

The reflectance, absorptance and transmittance profile of ZnO-Pt DSSC coupled with and without 1D SiO2/TiO2 PhC

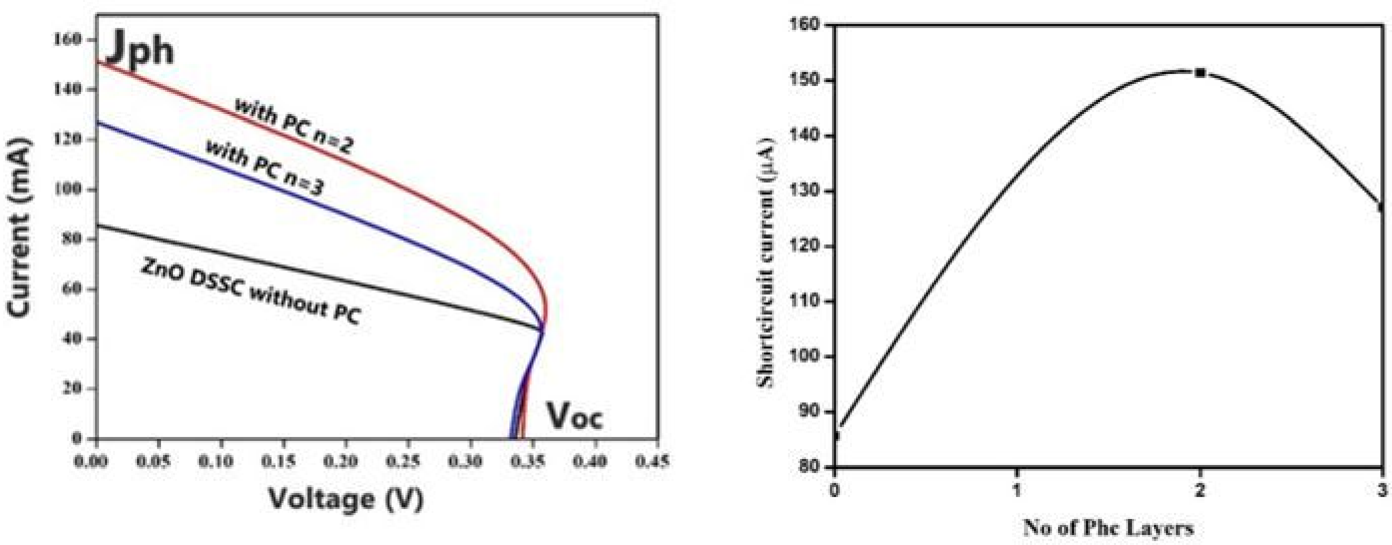

Figure 4

I-V curve and Photo current -vs number of periods of ZnO-Pt DSSC coupled with and without 1D SiO2/TiO2 PhC