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INVESTIGATING THE PERFORMANCE OF TiO2 AND ZnO BASED DYE-SENSITIZED SOLAR CELL

Md. Mohitul Haque[1], **Charles Dickens Tusha Falia**[2], **Mahmudul Hasan**[3]

[1,2,3]BSc in EEE, East West University, Bangladesh
ijenn.price@gmail.com[1], *tushafalia@gmail.com*[2], *tonmoy.bd@live.com*[3]

Abstract*- Generation of solar energy is steadily getting better over the decennaries and DSSC (dye-sensitized solar cell) can contribute majorly in the process as it approaches thin film technology that is highly effective. By addition of cells of distinct band gaps on a tandem cell's cell stack, efficiency can be improved. A double layered DSSC was analyzed in this work where composited photoanode ZnO and TiO2 were prepared on Tin Oxide (FTO) doped with Fluorine. For various thicknesses, wavelength and absorption coefficient, photovoltaic properties, J-V and I-V curve were assessed. Especially for thin films, higher intake contributes to greater J-V properties, according to the outcomes of experiment. Optimum thickness for wavelength of electromagnetic light wave was observed to be 300 to 400 nanometers and for thin film materials was 10 micrometers. Combining photoanode of TiO2 and compact layer of ZnO is observed to enhance J-V, I-V characteristics as well as absorption.*

Keywords: *DSSC, Solar energy, TiO2, ZnO, Fluorine-doped Tin Oxide*

1. INTRODUCTION

DSCC (Dye-Sensitized Solar Cell) or Grätzel Cell is the third-generation photovoltaic (PV) cell [1]. The silicon-based first-generation cell is costly but has an efficiency of 16-21% [1]. CdTe and amorphous silicon are the main basis of PV cells of the second generation with an efficiency of around 10-15% and the third-generation is cheap and is not acquainted with the theoretical perimeter of Shockley-Queisser where the other two generations have this limitation [1]. Here, we evaluated the performance of DSSC by utilizing a composite photoanode of TiO2 and compact layer ZnO on Fluorine-doped Tin Oxide. Also, we analyzed the thickness effect on DSSC, optical transmission spectrum analysis and J-V characteristics and performance analysis of the DSSC. All necessary simulations in this study were performed in MATLAB.

2. STUDY OF DSSC

The utilization of a compact layer in DSCC can enhance performance of solar cells. EHP recombination can reduce solar cell performance which is prevented by compact layer which is basically fabrication of Fluorine-doped Tin Oxide. In Fig. 1 we get the architecture of DSSC modeling.

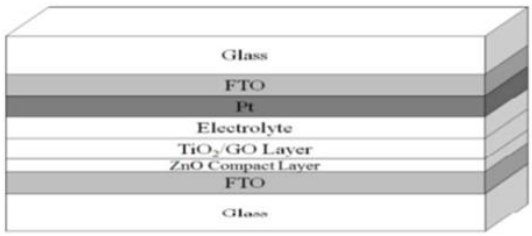

Figure 1: A DSSC structure with ZnO and TiO2 layers [2]

Table 1 displays ZnO nanotube and TiO2 nanostructure-based electrical parameters of DSSC.

Table 1: DSSC parameters used in the simulation

Parameters	ZnO nanotube	TiO2 nanostructures
I_{ph} (mA-cm^{-2})	3.36	16.88
Is (µA)	0.17334	0.34566
n	3.570858	1.639251
Rs(Ω)	0.393552	0.026832
G_{sh} (Ω^{-1})	0.000699	0.001378

2.1 Simulation and Discussion

Figure 2, 3 and 4 shows the I-V characteristics for TiO2, ZnO, and a combination of TiO2-ZnO, respectively. We get an open-circuit voltage of 0.46V for a short circuit current value of 0.016A which is shown in Fig. 2.

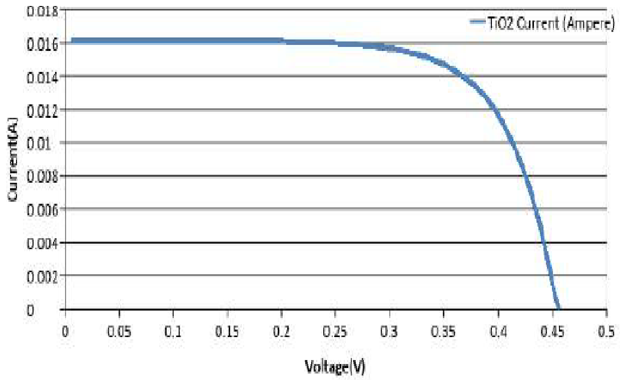

Figure 2: TiO2 layer I-V curve

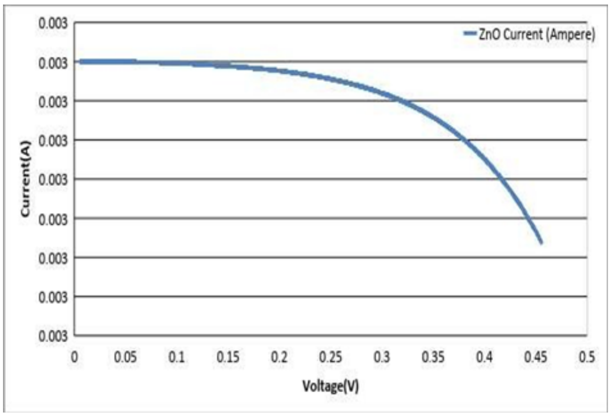

Figure 3: ZnO layer I-V curve

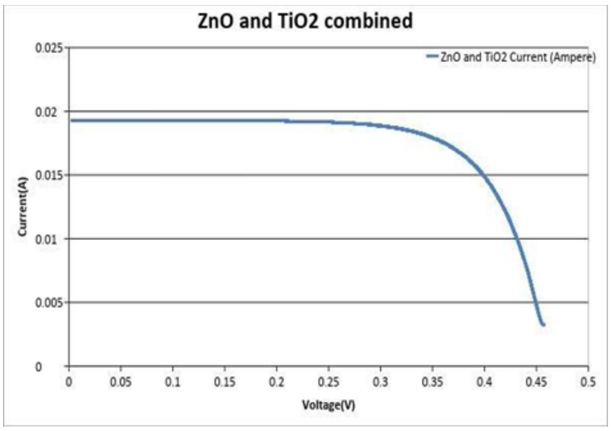

Figure 4: ZnO and TiO2 combination layer I-V curve

From the figures above, it was calculated numerically that the I-V features change considerably for the mixed layer of TiO2 and ZnO, where for the ZnO layer it decreases steadily from 0.003A. It is noted that the short circuit current rises to about 0.02A in Fig. 4, which is important. It is forecasted from the above figure that the voltage and current for the combined layer will rise.

3. STUDY OF THICKNESS EFFECT ON DSSC

Here, we will address the reliance on DSSC in film thickness. Some study articles recently used an electron diffusion-based mathematical model to study the impact of conductor thickness in DSSC [3, 4]. The diffusion sample utilizes distinct thicknesses to check dissimilarity in open-circuit voltage.

3.1 Modeling

Two equations were used by Sodergrenin in the model of his article to observe generation, recombination, and transport properties of the electron in thin-film nanostructure [5]:

$$\frac{\partial^2 n(x)}{\partial x^2}D-\frac{n(x)-n_0}{\tau}+\phi_0\alpha\exp(-\alpha x)=\frac{\partial n}{\partial t} \qquad (1)$$

Under steady-state eq.1 becomes [6]:

$$\frac{\partial^2 n(x)}{\partial x^2}D-\frac{n(x)-n_0}{\tau}+\phi_0\alpha\exp(-\alpha x)=0 \qquad (2)$$

Photocurrent can be simply extorted from electrons. Also as an opposite electrode, electrons were never drawn directly. Thus, the conditions of the boundary are given as:

$$n(0)=n_0 \quad \text{and} \quad \left.\frac{dn}{dx}\right|_{x=d}=0$$

The surplus concentration of electron of photovoltage, Vph is given by:

$$|V_{ph}|=\frac{kt}{q}m\ln\frac{n_{contact}}{n_0} \qquad (3)$$

The expression below can be used to calculate short-circuit current density [6]:

$$J_{sc}=\frac{q\phi L\alpha}{1-L^2\alpha^2}\left[-L\alpha+\tanh\left(\frac{d}{L}\right)+\frac{L\alpha\exp(-d\alpha)}{\cosh\left(\frac{d}{L}\right)}\right] \qquad (4)$$

Below boundary conditions can be found after resolving eq. 3 and eq. 2 that results in voltage and current:

$$V=\ln\left[1+\frac{(J_{SC}-J)L}{qDn_0\tanh\left(\frac{d}{L}\right)}\right]\frac{kTm}{q} \qquad (5)$$

This equation can be solved to yield:

$$J=J_{SC}-\frac{qDn_0}{L}\tanh\left(\frac{d}{L}\right)\left(\exp\left(\frac{qV}{kTm}\right)-1\right) \qquad (6)$$

3.2 Calculation of Internal parameter of DSSC

Five inner parameters of DSSC can determine the impacts of density on J-V features. These can be acquired from the material properties' practical values. In our modeling research, D in the value of mid-range is used, which is approximate $5.0\times10^{-4}cm^2s^{-1}$ [6].

3.3 Results and Discussion

From Fig. 5 it is evident that with rising thickness the density of current (Jsc) rises concurrently, although Jsc reduces gradually after reaching peak for the thickness of 10μm. The inner surface area expands as thickness rises which results in an elevated dye loading according to electron photogeneration [7]. The figure also displays open-circuit voltage declines as the conductor thickness increases as a dilution effect of electron [3, 4].

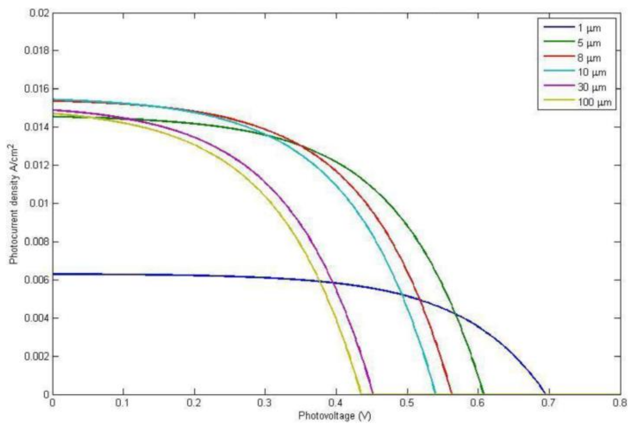

Figure 5: J-V curve for TiO2 thickness

From Fig. 6, we found that the current density reaches its peak at 0.00656 for 20μm thickness, where open-circuit voltage (Voc) is found to be 0.61V.

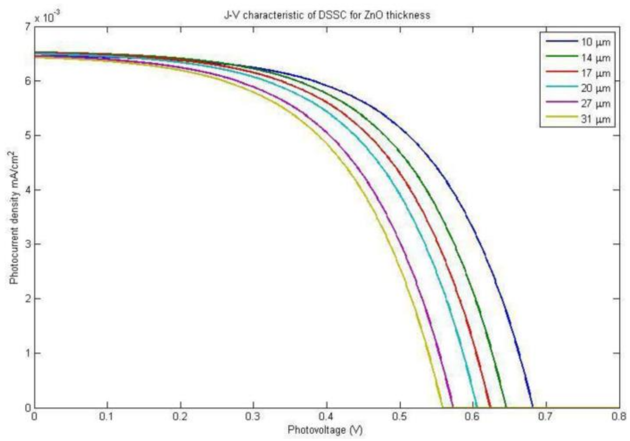

Figure 6: J-V curve for ZnO thickness

From Fig. 7 it is evident that maximum Jsc=0.0168 and Voc=0.73V are found at 10.25μm electrode thickness for TiO2 & ZnO combined. The voltage declines gradually for increasing conductor density but no prominent changes in Jsc are seen which can be explained by electron photogeneration.

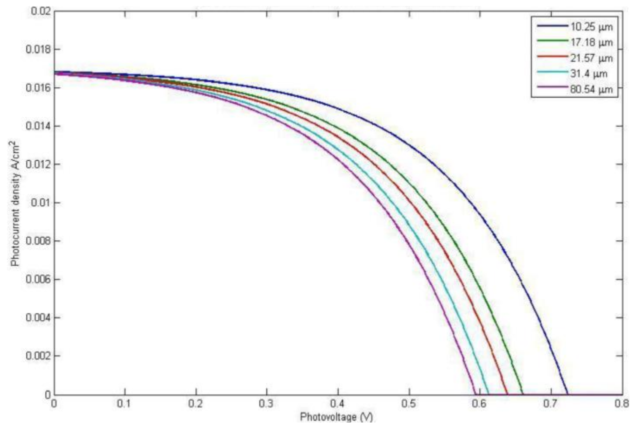

Figure 7: J-V curve for ZnO and TiO2 combination layer thickness

4. STUDY OF THICKNESS EFFECT ON DSSC

4.1 Spectrum of Optical Transmission

Semiconductors for DSSC (Dye-Sensitized Solar Cell) tend to have significant light absorption characteristics. For generating preferred reflectivity and transmitting properties, optical thin films are chosen by placing very thin layers on each other material or elements [7]. In this situation, the identical characteristics of absorption of light, specific materials with wide bandgap keep researchers attracted.

4.2 Short Revision of TiO2 and ZnO Properties

ZnO shows promising features for optical photo electrochemical conduct and reactions as it possesses a big bandgap of 3.37eV [8]. In this research, we explored ZnO film's absorbance conduct on N-BK7 optical glass for various wavelengths on spectrum of Ultraviolet-visible spectroscopy to comprehend light suction characteristics of ZnO film so that the most efficient difference in wavelengths can be optimized for absorbance to achieve the highest efficiency in DSSC layer building. We also explored TiO2 film's absorbance conduct on the glass known as Fluorine-doped Tin Oxide glass for various spectrums of Ultraviolet-visible spectroscopy wavelengths to know its absorption characteristics inherited especially in film of TiO2.

4.3 Obtaining Variable for Simulation

Air's Refractive index was fixed at 1.00 in every wavelength in Ultraviolet-visible spectroscopy. This formula has been used to calculate the reflection of TiO2 and ZnO thin film on Fluorine-doped Tin Oxide glass and N-BK7 optical glass, respectively, where Reff is the efficient reflection [9].

$$R_{eff} = \frac{P^2+Q^2+2PQ\cos R}{1+P^2Q^2+2PQ\cos R} \quad (7)$$

This formula was used to calculate the transmission of TiO2 and ZnO thin film on Fluorine-doped Tin Oxide glass and N-BK7 optical glass accordingly, where T_{eff} is the efficient reflection [7].

$$T_{eff} = \frac{16 n_0^2 n_f^2 n_s}{1+P^2Q^2+2PQ\cos R} \quad (8)$$

Using dispersion formula [8], glass's refractive indices values have been determined,

$$1-n^2 = \frac{\lambda^2 \times 1.03961212}{0.00600069897-\lambda^2} + \frac{\lambda^2 \times 0.231792344}{0.0200179144-\lambda^2} + \frac{\lambda^2 \times 1.01046945}{103.560653-\lambda^2} \quad (9)$$

Absorption coefficient (α) can be obtained through eqn. 10.

$$\alpha = \frac{1}{t} \ln \frac{(1-R)^2}{T} \quad (10)$$

Lastly, absorbance values for certain electromagnetic spectrum also called a spectrum of Ultraviolet-visible spectroscopy derived from eqn. 11 [10].

$$A = \frac{\alpha \times d_f}{2.303} \quad (11)$$

Figures 8 and 9 show the eventual absorbance for TiO2 and ZnO thin film on N-BK7 optical glass at the spectrum of Ultraviolet-visible spectroscopy.

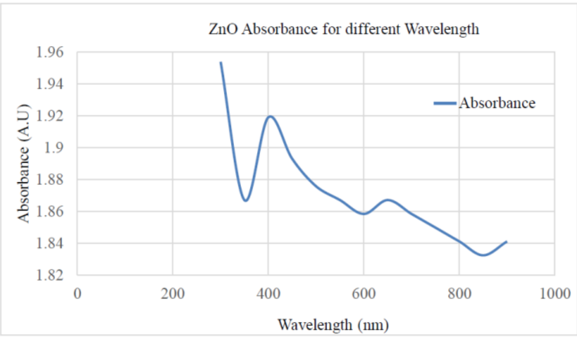

Figure 8: Absorbance vs. Wavelength for ZnO

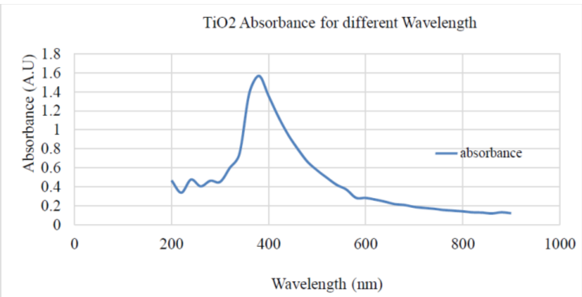

Figure 9: Absorbance vs. Wavelength for TiO2

From these figures, it is evident that thin film of ZnO experiences its peak absorbance 1.9539A.U. at 300nm (ultraviolet region), which means 0.2μm thin film of ZnO has an excellent feature to absorb specifically UV spectrum where TiO2 absorbs maximum radiation at the staring of ultraviolet region. Also absorbance of TiO2 is the lowest after 600nm and below 300nm. The absorbance range for TiO2 has been optimized between 300 nm and 600 nm.

5. J-V FEATURES WITH BEHAVIOUR ANALYSIS

5.1 Parameter Extraction for Simulation:

In the case of both materials, the value of n_0 is $1.10\times10^{16}\text{cm}^{-3}$

Temperature = 300K, for both materials

Coefficient of Absorption in ZnO (α) = [2240 2230 2209] (cm^{-1}) also the thickness of ZnO, d = 0.2 μm

Coefficient of Absorption in TiO2 (α) = [4497 6802 4278] (cm^{-1}) also the thickness of TiO2, d = 7.6 μm

ϕ(phi)= $1.00\text{x}10^{17}$ ($\text{cm}^{-2}\text{s}^{-1}$). [11]

5.2 Results of Comparative Simulation:

Figures 10 and 11 show the eventual J-V features of ZnO and TiO2 for a specific coefficient of absorption in different wavelengths, such as 600nm, 400nm, and 300 nm.

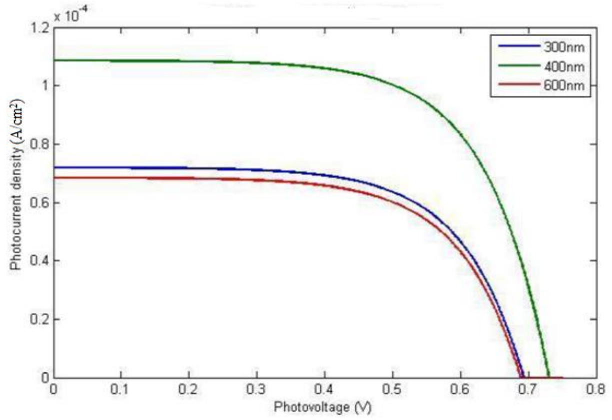

Figure 10: J-V curve for TiO2 in different wavelengths (Thickness 7.6 μm)

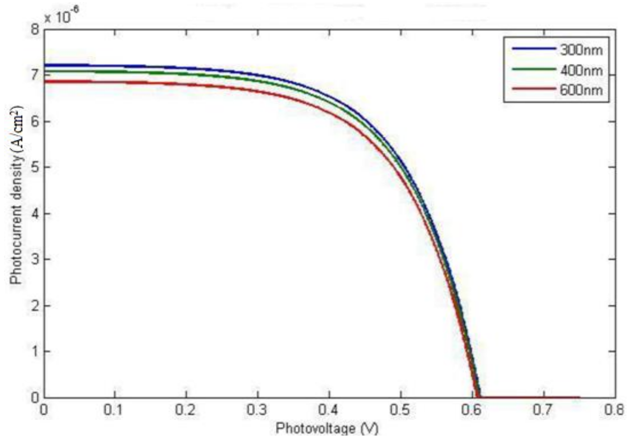

Figure 11: J-V curve for ZnO in different wavelengths (Thickness 0.2 μm)

Figures 12 and 13 show the eventual characteristics of J-V for the combination of ZnO and TiO2 (for thickness of

7.8µm and 10µm) for specific absorption coefficient of different wavelengths, such as 600nm, 400nm, and 300 nm.

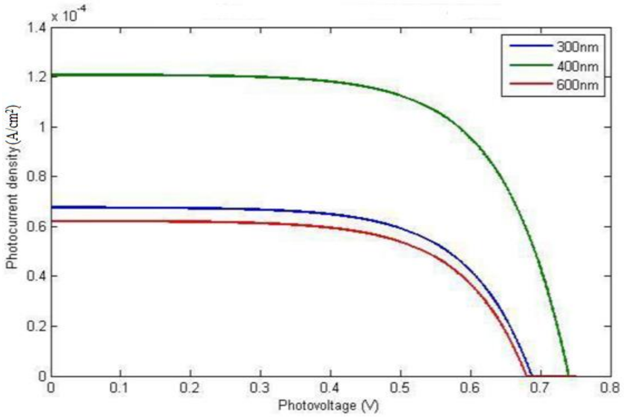

Figure 12: J-V curve for TiO2 and ZnO combined in different wavelengths (Thickness 7.8 µm)

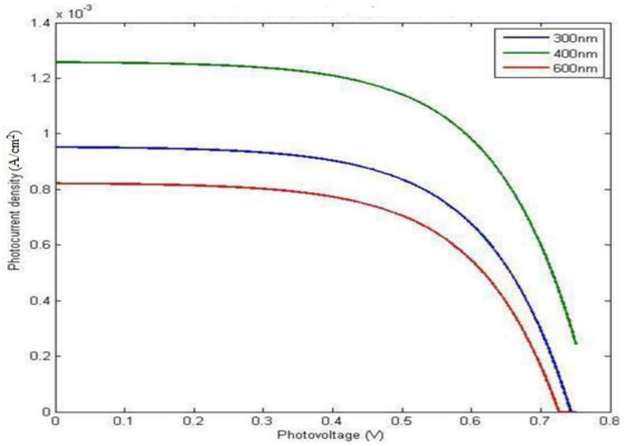

Figure 13: J-V curve for TiO2 and ZnO combined in different wavelengths (Thickness 10 µm)

5.3 Analysis and Discussion

Simulation results for specific wavelengths and thickness have been displayed in Table 2 and Table 3. From the results of our analytical comparison based simulation work, it can be summarized that the composition ZnO and TiO2 has the optimum absorbance characteristic on a wavelength scale of 380-400 nm where both V and J are important.

On the other side, mixed composite materials like TiO2 and ZnO combined have displayed that characteristics for absorbing specific ranges of UV spectrum along with visible spectrum differ from one another. Both TiO2 and ZnO's high bandgaps have the benefits of absorbing the various areas of ultraviolet electromagnetic wavelength light where ZnO has shown more absorption of visible light as well as a comparative advantage in absorbing infrared light. For improving J-V characteristics, layer diffusion is of tremendous significance to each other although other coefficients and variables such as density, electron diffusion duration can influence strongly to evaluate J-V performance.

Table 2: Simulation result for specific wavelengths

Wavelength (nm)	ZnO and TiO2 (V, J), (V, Acm^{-2}) 7.8µm of thickness	ZnO (V, J), (V, Acm^{-2}) 0.2µm of thickness	TiO2 (V, J), (V, Acm^{-2}) 7.6µm of thickness
300	0.69, 0.69×10^{-4}	0.615, 7.24×10^{-4}	0.685, 0.735×10^{-4}
400	0.745, 1.215×10^{-4}	0.61, 7.16×10^{-6}	0.735, 1.1×10^{-4}
600	0.685, 0.625×10^{-4}	0.608, 6.86×10^{-6}	0.68, 0.685×10^{-4}

Table 3: Simulation result for specific wavelengths in 10µm of thickness

Wavelength (nm)	ZnO (V, J), (V, Acm^{-2})	TiO2 (V, J), (V, Acm^{-2})	ZnO and TiO2 (V, J), (V, Acm^{-2})
300	0.725, 0.62×10^{-3}	0.77, 6×10^{-4}	0.745, 0.94×10^{-3}
400	0.757, 0.88×10^{-3}	0.764, 7.68×10^{-4}	0.775, 1.27×10^{-3}
600	0.71, 0.76×10^{-3}	0.7632, 7.65×10^{-4}	0.725, 0.819×10^{-3}

6. CONCLUSION

In this work, we studied the optimized thickness required to improve J-V characteristics together with the resulting absorption coefficient obtained from the properties of absorbance vs. wavelength. By performing simulation, we apprehended that for thin films, in particular, greater absorption results in greater J-V features. To enhance J-V performance, the optimal thicknesses detected were 10 and 27 micrometers for TiO2 and ZnO, respectively and for both combinations, the optimal thickness observed was 10.25mm. In terms of enhancing J-V and I-V characteristics and absorption in respective areas, photoanode of TiO2 and compact layer of ZnO combined experienced important variations.

7. REFERENCE

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8. NOMENCLATURE

Symbol	Meaning	Unit
I	Current	(A)
V	Voltage	(V)
J	Current Density	(Acm^{-2})
R	Resistance	(Ω)
ϕ	Light intensity	($cm^{-2}s^{-1}$)
D	Diffusion coefficient	(cm^2s^{-1})
α	Light absorption coefficient	(cm^{-1})
m	Ideality factor	(Dimensionless)
t	Electron lifetime	(ms)
L	Electron diffusion length	($cm^{-1}s^{-1}$)
d	Thickness of Film Thickness	(μm)
λ	Wavelength	(nm)