Accepted Manuscript

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Manuscript number**: PCCC-2506-1400**

To appear in: Progresss in Color, Colorants and Coatings

Received: 30 May 2025

Final Revised: 10 July 2025

Accepted: 12 July 2025

Please cite this article as:

Abdelkhalk Aboulouard, Mohamed Jouaiti, Mohammed El Idrissi, Simulation analysis of dye-sensitized photovoltaic cells performance using three moroccan natural dyes, Prog. Color, Colorants, Coat., 19 (2026) XX-XXX.

DOI: 10.30509/pccc.2025.167563.1400

Simulation Analysis of Dye-Sensitized Photovoltaic Cells Performance Using Three Moroccan Natural Dyes

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Abstract

In recent years, increasing focus on environmental sustainability and the circular economy has sparked a resurgence of interest in incorporating eco-friendly and recyclable materials across numerous industries. Creating advanced dye-sensitized solar cells (DSSCs) employing natural dyes has a significant impact in fulfilling the need for environmentally sustainable technologies. In this study, we use MATLAB to examine the electrical features of DSSCs. The study relies on a model of electron diffusion in a porous titanium dioxide thin film and the absorption coefficient of local dyes. These latter are extracted from grapes, pomegranates and Moroccan roses. In particular, we investigate the absorbance of pigments by a spectrophotometer and the electrical features of DSSCs. The findings indicate that the photovoltaic performance metrics, such as maximum power voltage, short-circuit current density, open-circuit voltage, and maximum power current, are superior for pomegranate dye compared to grape and Moroccan rose dyes. This superiority is attributed to the higher absorption coefficient of the pomegranate dye, which efficiently absorbs incident light and generates excitons.

Keywords: Dye-sensitized solar cells; natural dyes; Matlab; photovoltaic performance; solar cells.

1. Introduction

Recently, the field of photovoltaic cells has advanced to transform sunlight into electricity. In this field, we focus on dye-sensitized solar cells (DSSCs), which are easy to manufacture and more environmentally friendly in contrast to alternative solar cell technologies [1]. The components of DSSCs include a semiconductor photoelectrode, counter electrode, electrolyte, and dye. Researchers have dedicated several efforts to enhancing the efficiency of DSSCs by studying each component.

For the semiconductor photoelectrode, many synthesis methods have been examined to synthesize and control the shape and size of the semiconductor. Titanium dioxide (TiO_2)

is the most commonly used semiconductor as a photoelectrode due to its good surface area and stability [2]. Among the synthesis methods, we found flame spray pyrolysis, hydrothermal sol-gel [3]. Various types of semiconductor structures were manufactured, such as nanofibers, nanowires, nanoparticles and nanotubes [2]. Moreover, platinum is extensively used as a counter electrode because of its good catalytic characteristics and electrical conductivity. As an alternative to platinum, some researchers have used carbon materials because of their low cost and resistance to corrosion [4]. Furthermore, the most commonly employed electrolyte in DSSC is iodide/triiodide because of its good redox potential but the main problems of this electrolyte are the leakage and volatility. As a solution, cobalt complexes, which have a higher redox potential, were used and showed an enhancement in the performance of cells [5]. The final component is the dye. This latter could be artificial or natural such as plants, fruits and roots. The metal-free organic and complex dyes are extensively used in DSSC because of their good spectral response into visible region [6].

In addition, many researchers have used natural dyes on DSSCs to reduce the manufacturing price and the environmental toxicity [7]. Furthermore, H. Bashar et al used red and green dyes, which are extracted from beetroot and spinach, respectively [8]. The power conversion efficiencies (PCE) reported are 0.56% for beetroot and 0.49% for spinach. Similarly, F. Kabir et al. used malabar spinach and red spinach as sensitizer and found PCE= 0.466% and PCE= 0.531%, respectively [9]. A simple cold and Soxhlet extraction method has been used to extract dyes from the dried leaves of indigo but the efficiencies achieved are low [10]. Many factors may affect the extraction of dye such as temperature, pH and various organic solvents. Mahmoud A.M. Al-Alwani et al. have studied the effect of these factors on the extraction of dye from Areca catechu [11]. The optimal dye extraction conditions were pH 10, 80 °C and ethanol as a solvent for extraction. However, the efficiency of these cells is not that much significant in comparison to cells based on artificial dyes because of their short spectral response and stability in the visible range. That's why many recent studies have been examined various natural dyes in order to improve the efficiency [12, 13].

From this standpoint, this paper aims to participate in these studies through a numerical and experimental method based on the absorption coefficient of the extracted local dyes. This approach is grounded in a framework that explains the photoelectrochemical behavior of DSSCs. For this purpose, three local Moroccan dyes have been extracted from pomegranate, grape and Moroccan rose. This study's novel contribution lies in the comprehensive analysis of the electrical features of DSSCs using Matlab simulations, specifically focusing on dyes derived from local Moroccan natural sources. The standout finding is the superior photovoltaic performance of pomegranate dye, which surpasses that of grape and Moroccan rose dyes. This is attributed to its higher absorption coefficient and the presence of anthocyanins, which enhance the transfer of electrons into the TiO_2 conduction band. Such insights provide a more thorough insight into the possibilities of natural dyes in improving DSSC efficiency.

2. Experimental

2.1. Extraction method of natural dyes

Samples of grape, moroccan rose and pomegranate were extracted. For this purpose, 7g of each sample was ground in a mortar with distilled water. 1 v/v of this solution is added to 25 ml of ethanol for two hours. After that, we collect the final solution after filtration with a funnel and filter paper. A UV-visible spectrophotometer will measure the absorbance of each dye to define the intensity for different wavelengths λ (the wavelengths λ were between 400 and 600 nm). The different dyes were stored under the same conditions in the dark to prevent them from being exposed to light.

2.2. Simulation method

Matlab was used to conduct the simulation. The work was performed under steady-state conditions of irradiated DSSCs. The excited dye injects electrons into the porous TiO_2 thin film and the recombination with the electrolyte will take place at the interface of TiO_2/electrolyte. The process is presented by this differential equation 1 [14]:

$$D\frac{\partial^2 n(x)}{\partial x^2} - \frac{n(x) - n_0}{\tau} + \phi\alpha\, exp(-\alpha\, x) = 0 \quad (1)$$

Where, D is the electrons diffusion coefficient, n(x) is the excess electrons generated, n_0 is the concentration of electrons in the dark under steady conditions, τ is the electron life time, α is the light absorption coefficient and Φ is the light intensity.

The probability of electrons being trapped- detrapped has not been considered in equation 1 since it is relevant just beneath non-stable conditions. Electrons are extracted as photocurrent under short-circuit conditions and the electrons are not directed to the counter electrode. Thus, the boundary conditions are given in equations 2 and 3:

$$n(0) = n_0 \quad (2)$$

$$\left(\frac{dn}{dx}\right)_{x=d} = 0 \quad (3)$$

Where d is the thickness of the electrode.

Therefore, the short-circuit current density J_{SC} can be presented as equation 4.

$$J_{SC} = \frac{q\phi L\alpha}{1-L^2\alpha^2}\left(-L\alpha + tanh\left(\frac{d}{L}\right) + \frac{L\alpha e^{-d\alpha}}{cosh(\frac{d}{L})}\right) \quad (4)$$

where, q is the electron charge and L is the length of electron diffusion presented as Equation 5.

$$L = \left(D\tau\right)^{1/2} \quad (5)$$

If the DSSC is operated at a determined potential difference between the potential redox electrolyte and the TiO_2 Fermi level, the electron density of the TiO_2/ transparent conductive oxide interface (x = 0) increments to n, providing a novel condition of the boundary (Eq. 6):

$$n(0) = n \quad (6)$$

The J-V relation can be described as (Eq. 7):

$$V = \frac{KTm}{q} ln\left(\frac{L(J_{SC} - J)}{qDn_0 \, tanh(\frac{d}{L})} + 1\right) \quad (7)$$

The input parameters were taken from the literature and shown in Table 1.

Table 1. Input factors.

Inputs	Value	Name	References
q	1.60218×10^{-19} C	Electron charge	
K	1.38066×10^{-23} J/K	Boltzmann constant	
d	5×10^{-4} cm	TiO_2 length	[14]
m	4.5	Ideality factor	[15, 16]
D	5×10^{-4} cm^2s^{-1}	Coefficient of diffusion	[14]
$\mathbf{n_0}$	5×10^{16} cm^{-3}	Electron concentration	[17, 18]
τ	0.01 s	Life time	[15, 19]
ϕ	10^{17} $cm^{-2}s^{-1}$	Light intensity	[15, 16]
T	300 K	Temperature	[20]

3. Result and Discussion

3.1. UV-Vis absorption of the dyes

A UV-Visible spectrophotometer was employed in order to establish the intensity of the absorbance light for the different samples. The grape absorption spectrum presented in Figure 1 can show a maximum absorption peak at 400 nm with an absorption region from 360 to 500 nm (Figure 1a). For pomegranate, the maximum absorption peak is at 500 nm with an absorption region from 400 to 600 nm (Figure 1b). For Moroccan rose, the maximum absorption peak is at 450 nm with an absorption region from 400 to 500 nm (Figure 1c). The spectrum of the different natural dyes strongly depends on the ethanol used for the extraction. The maximum absorbances of UV spectra were found between 400 and 500 nm, which is a direct result of the presence of phenolic groups. Phenolic compounds are known for their great absorption in the UV-visible region, primarily due to their conjugated double bond systems and aromatic ring structures. These features allow phenolic compounds to absorb light energy efficiently, elevating electrons from the highest occupied molecular orbital (HOMO) to the lowest unoccupied molecular orbital

(LUMO). Specifically, anthocyanins, a class of phenolic compounds abundant in pomegranates and grapes, are responsible for their vibrant colors [9, 21, 22].

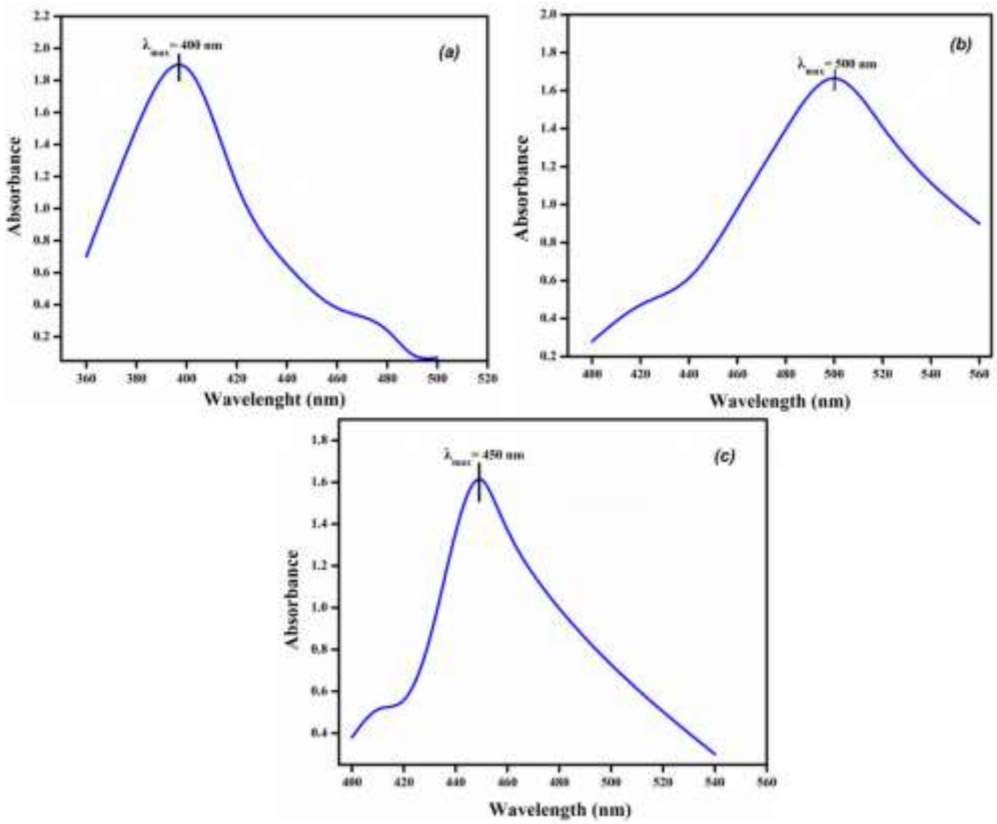

Figure 1. UV-Vis absorption spectrum of the dyes (a) grape, (b) pomegranate, and (c) Moroccan rose.

The amount of light absorbed indicates the absorption coefficient. The Beer-Lambert Law allows for the absorption coefficient to be obtained at the corresponding wavelengths. The equations 8 and 9 represent this law [23]:

$$A = k.c \tag{8}$$

$$A = \alpha.l.c \tag{9}$$

where, A is the absorbance, k is the proportional coefficient, c is the concentration of the pigments, l is the length of the optical direction, and α is the absorption coefficient.

Table 2. Absorption coefficient and proportional coefficient of samples.

Pigments	Proportional coefficient (L/mol^{-1})	Optical path length (cm)	Absorption coefficient (L/mol^{-1} cm^{-1})
Grape	18.019	1.2	15.016
Pomegranate	29.871	1.2	24.89
Moroccan rose	3.2	1.2	2.667

The higher value of the absorption coefficient that can be seen in Table 2 signifies that the pomegranate absorbs the incident light with an enormous wavelength. If the absorbed wavelength increases, the energy of the photon needed to stimulate the electron's transition from the HOMO to the LUMO is decreased, which permits to introduce the electrons easily into the TiO_2 band conduction. The high absorption coefficient value could improve the performance of DSSCs.

3.2. Electrical performance

The simulation of electrical characteristics such as maximum power voltage (V_{mp}), J_{SC}, open-circuit voltage (V_{oc}), maximum power current (J_{mp}), and power (P) was performed on MATLAB by using the absorption coefficient of grape, pomegranate, and Moroccan rose. The results of the simulation are shown in Figures 2 and 3.

Table 3. Electrical performance parameters of DSSCs employing natural dyes from pomegranate, Moroccan rose, and grape.

Dye	Short-Circuit Current Density (JSC, mA/cm²)	Open-Circuit Voltage (Voc, V)	Maximum Power Current (Jmp, mA/cm²)	Maximum Power Voltage (Vmp, V)	Power (P, $\times 10^{-4}$ W)
Pomegranate	0.195	0.144	0.113	0.083	93.7
Moroccan Rose	0.021	0.027	0.010	0.014	1.529
Grape	0.118	0.106	0.066	0.059	38.84

Nevertheless, the electrical performance metrics for DSSCs using pomegranate, Moroccan rose, and grape dyes are presented in Table 3. Pomegranate has excellent photovoltaic performance compared with the grape and Moroccan rose. This is attributed to a more significant absorption coefficient. This higher absorption leads to a more efficient generation of electron-hole pairs, thereby enhancing the short-circuit current density and overall efficiency of the DSSC. Furthermore, anthocyanins in pomegranate are known to have strong electron-donating properties due to their hydroxyl and methoxy groups, which facilitate efficient electron injection into the TiO_2 conduction band. The structure of anthocyanins allows for better alignment and interaction with the TiO_2 surface, enhancing the charge transfer process and reducing recombination rates. This leads to improved photovoltaic performance [9, 21, 22, 24]. A manner of enhancing the DSSC performance is to blend certain natural dyes as a cocktail to enhance the dye absorption coefficient [8, 9, 25].

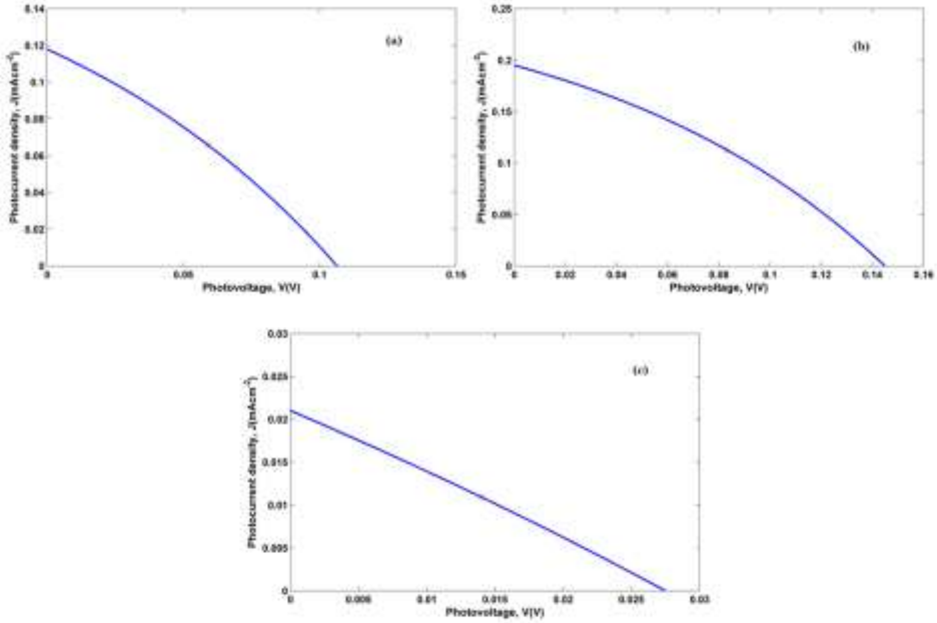

Figure 2. J-V curves of the extracted dyes (a) grape, (b) pomegranate, and (c) Moroccan rose.

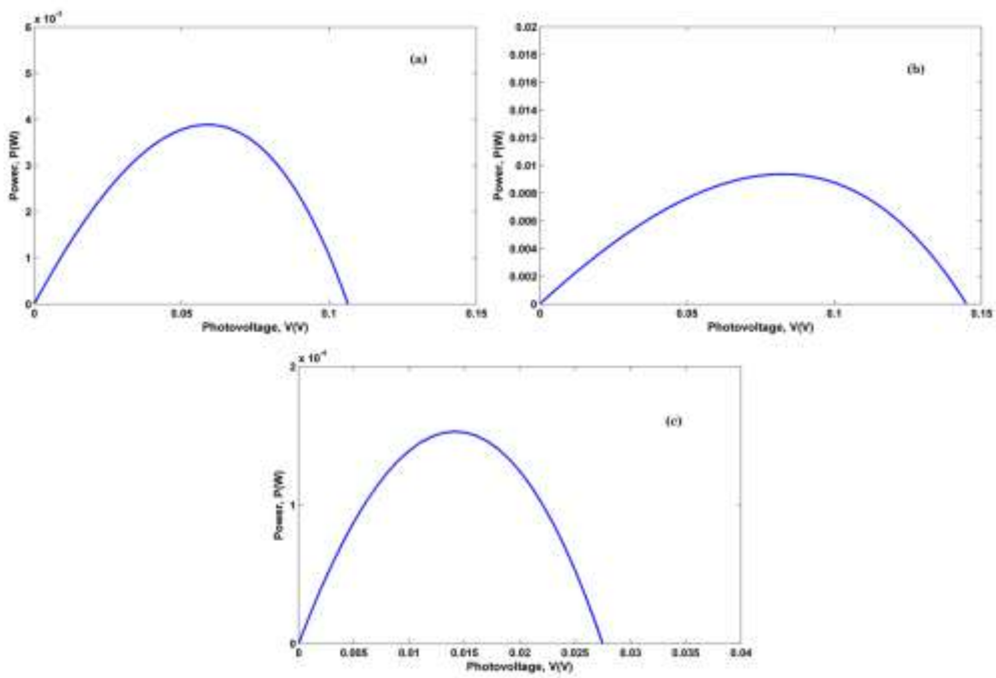

Figure 3. P-V curves of the extracted dyes (a) grape, (b) pomegranate, and (c) Moroccan rose.

4. Conclusion

In this work, a numerical simulation was carried out to study the electrical features of the DSSC. Firstly, the dyes have been extracted from three natural pigments. The pigments are grape, Moroccan rose, and pomegranate. The purpose of the extraction is to determine the absorption coefficients of each dye experimentally. Secondly, the coefficients are used in the simulation program to determine the electrical characteristics of DSSCs. As a result, J_{SC} = 0.195 $mAcm^{-2}$, V_{oc} = 0.144 V, J_{mp} = 0.113 $mAcm^{-2}$, V_{mp} = 0.083 V, P = 93.7×10^{-4} W for pomegranate, J_{SC} = 0.021 $mAcm^{-2}$, V_{oc} = 0.027 V, J_{mp} = 0.01 $mAcm^{-2}$, V_{mp}= 0.014 V, P= 1.529×10^{-4} W for Moroccan rose, J_{SC} = 0.118$mAcm^{-2}$, V_{oc} = 0.106 V, J_{mp} = 0.066 $mAcm^{-2}$, V_{mp} = 0.059V, P = 38.84×10^{-4} W for grape. We figured out that pomegranate has a good photovoltaic characteristic compared to grape and Moroccan rose. This enhanced performance is attributed to the higher absorption coefficient of pomegranate dye, which allows for more efficient light absorption and exciton generation. Future work will focus on exploring other natural dyes to enhance the electrical characteristics of DSSCs further. This study contributes to research on advancing sustainable energy solutions by utilizing natural, eco-friendly materials.

Acknowledgments: Gratitude is extended to the unidentified reviewers whose insightful feedback and recommendations greatly contributed to the improvement of this work**.**

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