

COMPUTATIONAL DESIGN OF NOVEL COUMARIN SENSITIZERS TO IMPROVE THE EFFICIENCY OF SOLAR CELLS

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Abstract

Abstract Dye Sensitized Solar Cells (DSSCs) are the most efficient third-generation solar cell to use because they have good chemical stability, low production cost, and environmental-friendly. Dyes have an important role on DSSCs, which is functioned as sensitizer (light-sensitizer). In this study, the modification of dyes was performed to produce a better light-absorption value. This study analyzed the D- π -A type of dyes (Donor- π conjugation-Acceptor) with coumarin donor and formic acid acceptor, then the π -conjugation was varied with butadiene, dicyclopentadiene, dipirol, difuran, and dithiophene molecules which later symbolized as dyes 1, 2, 3, 4, and 5. This study used Gaussian 16W program packaged with DFT (Density Functional Theory) and TD-DFT (Time Dependent-DFT) measurement methods as well as B3LYP/6-31G Basis Set. The analysis descriptors were HOMO (Highest Occupied Molecular Orbital) and LUMO (Lowest Unoccupied Molecular Orbital) energies, band gap (ΔE), HOMO and LUMO contours, excitation energy (E_{eks}), excitation wavelength (λ_{eks}), oscillator strength (f) and LHE (Light Harvesting Efficiency). The measurement results showed that all dyes were capable of absorbing light into the visible light area and the dye 3 produced the light absorption on the longer wavelength. It has been concluded that coumarin-based D- π -A type of dyes can improve the efficiency of light absorption on DSSCs.

Keywords: DSSCs, D- π -A Type, Coumarin, DFT/TD-DFT,

1. Introduction

Dye Sensitized Solar Cells (DSSCs) offer an efficient and easy-to-implement technology for the supply of energies in the future due to unlimited resources, providing materials efficiency, easy to be produced, low production cost and eco-friendly[1]. The main components of DSSCs consist of TiO₂ electrode, sensitizer, and I⁻/I₃⁻ electrolyte. Dyes are used as the sensitizer that have important contributions to improve the efficiency of the light absorption of solar cells[2]. There are two types of sensitizer that can be used, i.e. the sensitizer from inorganic dyes and the sensitizer from organic dyes[3]. Inorganic sensitizers have widely used, one of them is the ruthenium-bipyridine complex which indicates that 11% of the conversion efficiency value is feasible to be used as the sensitizer on DSSCs[4]. However, these dyes have limitations on their sources while also causing impacts on the environment, so did the previous study that used zinc-porphyrin complex which also has good efficiency on DSSCs but gained issues on the low synthesis result and poisonous materials for the synthesis process[5]. Organic sensitizers have advantages, i.e. low cost, good flexibility, high molar coefficient, and cause no impact on the environment⁶. Unfortunately, organic dyes are yet to produce the high efficiency of light absorption. Therefore, experimental and computational studies on the modification of D- π -A (Donor- π conjugation-Acceptor) system of dyes thrive[7-10], D-D- π -A, D-A- π -A, D-(π -A)₂, (D- π -A)₃L₂, D- π -A- π -A, D-A with good efficiency of light absorption due to the push-pull effect [11-16]. These dyes have the push and pull electronic nature, thus, they can cause the occurrence of the electron resonance of π -conjugation. A longer resonance of π electron will make the light to be absorbed on a longer wavelength (red shift). Computational study plays the role in substantiating the synthesis of dyes experimentally because the calculation of effective quantum predicts the physical and chemical properties of a compound [17]. Density Functional Theory (DFT) is widely used as the standard computational method for optimization due to its accurate measurement that is compatible with the experiment result [10]. According to the description above, the author was evoked to conduct a study concerning organic dyes of D- π -A type with coumarin framework by applying DFT measurement method. Coumarin was used as the donor chain and formic acid worked as the acceptor with π chain variations, such as butadiene, dicyclopentadiene, dipirol, difuran, and dithiophene. The D- π -A was selected due to its simpler structure. This study is expected to provide information regarding the most efficient structure of dyes to be used as the sensitizer on DSSCs instruments in the future, therefore, it can be made as the basis to synthesis such compound experimentally.

2. Materials and methods

The molecule structure was made with Gauss View 6.0. The molecule model in this study was coumarin-based D- π -A type of dyes with the framework as follows:

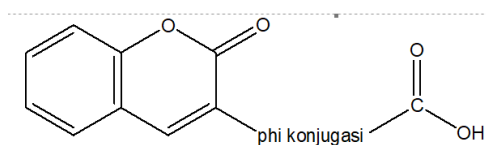


Figure 1. The molecule basic structure of Coumarin-based D- π -A type of dyes with π -conjugation variation chains

2.1 The variation chains of π -conjugation

The π -conjugation of the dyes in Figure 2 were varied with some structures described as follows:

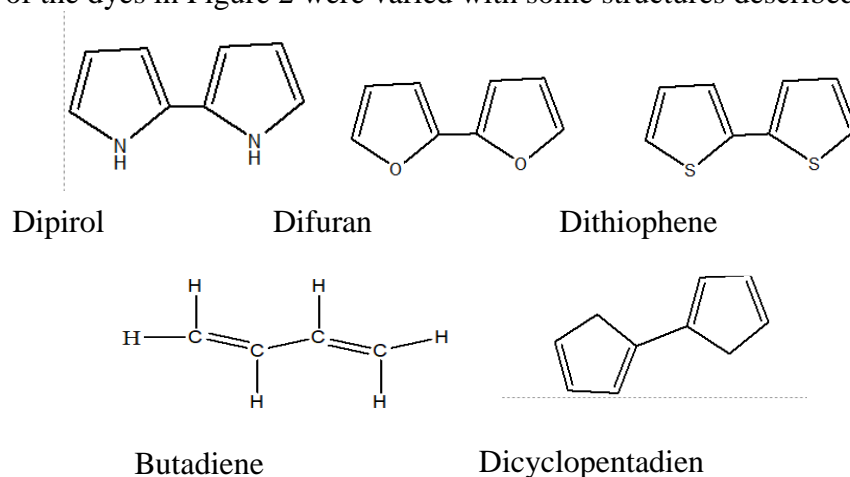


Figure 2. The structure variation of π -conjugation chains

2.2 The addition of electron donating and withdrawing groups

The effect of electron withdrawing and donating groups on organic dyes. The optimal dyes were added with electron withdrawing and donating groups, and be compared on their effect toward the addition of such groups.

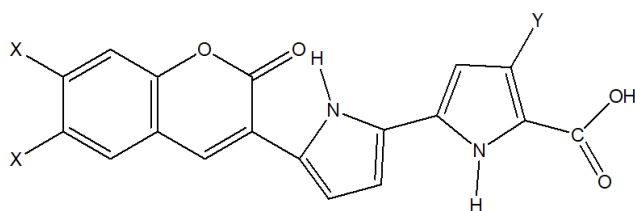


Figure 3. The molecule structure of dyes based on the substituent addition of electron donating (X) and withdrawing (Y) groups on organic dyes

According to the chain variation of π , the dye providing the best light absorption was added with electron withdrawing group, i.e. $-\text{NO}_2$, and electron donating group, i.e. $-\text{C}_2\text{H}_5$.

2.3 The optimization of D- π -A Type of Dyes with Aniline chain

The molecule structure of D- π -A type of dyes was drawn in the program using Gauss View 6.0 which later be performed with the geometric structure optimization. The entire input files of coumarin-based dyes were optimized by using Gaussian 16W program. The geometric optimization of molecule used DFT method and the optimization of molecule in the excitation state used TD-DFT method (Time Dependent-Density Functional Theory) with B3LYP/6-31G basis set [18,19].

2.4 Data Analysis

The optimal organic dyes then be analyzed on their values of electronic parameters, including E_{HOMO} , E_{LUMO} , band gap (ΔE), HOMO and LUMO contour, optical parameters, i.e. absorption spectrum, excitation

energy, excitation wavelength (λ_{eks}), oscillator strength (f) and LHE (light harvesting efficiency) and electrical parameters, i.e. current density (J_{sc}), voltage (V_{OC}) and energy conversion efficiency (η)

Some formulas used for the data analysis are as follows:

$$\text{Band Gap } (\Delta E) = E_{\text{LUMO}} - E_{\text{HOMO}} \quad (1)$$

$$\text{LHE} = 1 - 10^{-f} \quad (2)$$

$$\eta = J_{\text{sc}} V_{\text{oc}} (ff) / I_s \quad (3)$$

$$J_{\text{sc}} = \int \text{LHE}(\lambda) \Phi_{\text{inject}} \eta_{\text{collect}} d\lambda \quad (4)$$

$$V_{\text{oc}} = E_{\text{LUMO}} - E_{\text{CB}} \quad (5)$$

In which:

E_{CB} = conduction band energy $\text{TiO}_2 = -0.4 \text{ eV}$

E_{LUMO} = LUMO energy of dyes

ff = fill factor

Φ_{inject} = electron injection efficiency

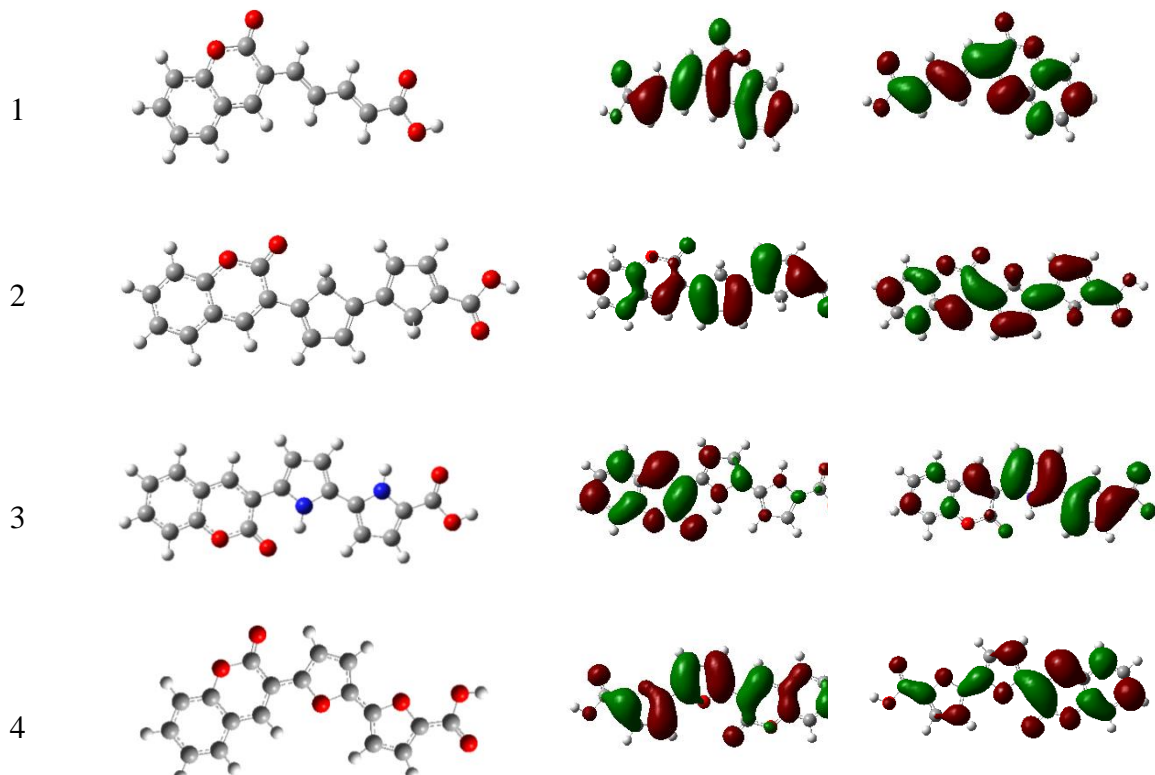
η_{collect} = charge collection efficiency [21-21]

according to the parameters mentioned above, the efficiency analysis of dyes as the sensitizer on DSSCs was performed.

3. Results and discussions

3.1 Optimal Geometric Structures

The structures were optimized from the basic state of the five dyes of π -conjugation chain variations. The geometric optimization was done to acquire the optimal molecular structures. The optimal structures, HOMO and LUMO contours of dyes 1, 2, 3, 4, 5 are shown in Figure 4.



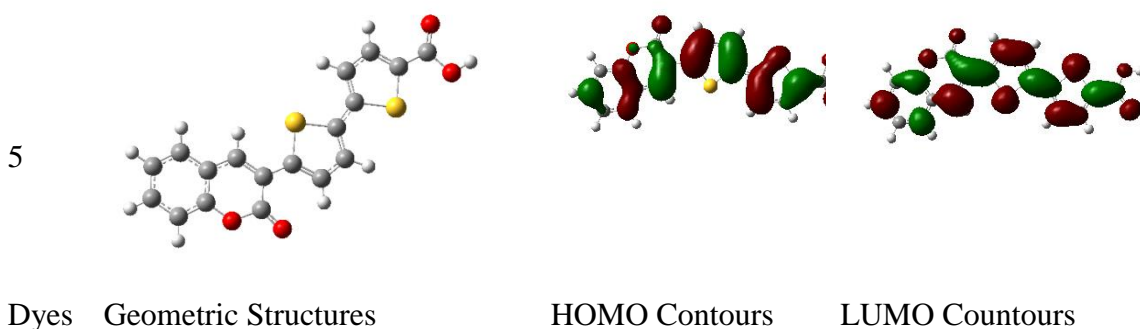


Figure 4. Optimal geometric structures, HOMO and LUMO contours of dyes 1-5 in which oxygen atom (red), Carbon (grey), Nitrogen (blue), Sulfur (yellow), Hydrogen (white)

HOMO band is electron-donating type while LUMO band is electron acceptor. Ideally, HOMO contour should be around the donor group and LUMO contour should be around the acceptor group [22,18]. Of HOMO contour, it was known that the electron donating group is coumarin and of LUMO contour, it was known that formic acid is electron acceptor. HOMO contour is in the π bond of donor chain and π conjugation, while LUMO contour is in the π bond of acceptor chain.

3.2 Bandgap (ΔE)

The difference between the energy level of HOMO and LUMO is mentioned as ΔE . HOMO as the molecular orbital that inhabited by the electron with the highest energy (valence band). LUMO is the molecular orbital that uninhabited by the electron with the lowest energy (conduction band). Bandgap are important factors in determining charge transfer from donors and acceptors chains[23] . According to the Planck's law, a lower ΔE means that the light will be absorbed on the longer wavelength, a longer wavelength means that more light can be absorbed by DSSCs. This condition occurs because an electron will move easier from one orbital with low energy level to the orbital with higher energy level, therefore, the sensitivity toward the light will also increase. The measurement results are presented in Table 1.

Table 1. The measurement results of the frontier energy of the optimization of dyes

Dyes	E_{Homo} (eV)	E_{Lumo} (eV)	ΔE (eV)
1	-6.0137	-3.1973	2.8164
2	-5.0589	-2.8749	2.1839
3	-4.9862	-2.6988	2.2874
4	-5.4986	-2.8425	2.6561
5	-5.5985	-3.0613	2.5372

From Table 1, it can be seen that dyes 2, 3, 4, and 5 have lower ΔE compared to dye 1. Based on the molecular structures, dyes 2, 3, 4, and 5 have a lot of π -conjugation electrons that resonate longer from the donor to acceptor chains, a longer resonance of electron of a dye; a red-shift will occur as the shift of absorption on the longer wavelength. Dye 2 had lower band gap compared to dyes 3, 4, and 5 because it molecules tend to be more planar so the resonance of π electrons on dyes happens quicker. Dyes 3 and 5 have atoms N and S in π chain in which atoms N and S have lower electronegativity compared to atom O in

the acceptor group (formic acid), therefore, electrons were easier to be withdrawn by atom O that was more electronegative [19], however, atom S had bigger molecules than atom O, thus, the electron withdrawing was weaker so the band gap of dye 5 was greater than dye 3. Dye 4 had a greater band gap because atom O existed in the π chain which also existed in donor and acceptor chains, therefore, the electron withdrawing power tends to be weaker. For the electron injection to happen more efficient within the cells, thus, E_{HOMO} values should be lower than the value of redox potential; I^-/I_3^- (-4.80 eV), therefore, it eases the transfer of electron from the electrolyte to the hole of dyes and the E_{LUMO} values should be higher on the conduction band; TiO_2 ($E_{\text{CB}} = -4.0$ eV) [21,22]. The data in Table 1 show that all dyes have lower than -4.8 eV E_{HOMO} and the closest to the value is dye 3. The E_{LUMO} values of all dyes are also higher than E_{CB} and the closest one is the E_{LUMO} of dye 3. This condition shows that the transfer of electrons within the cells occurs quicker by the presence of dye 3.

3.3 The adsorption spectrums

The adsorption spectrums of dyes 1-5 are shown in Figure 5 and the electronic transitions are shown in Table 2.

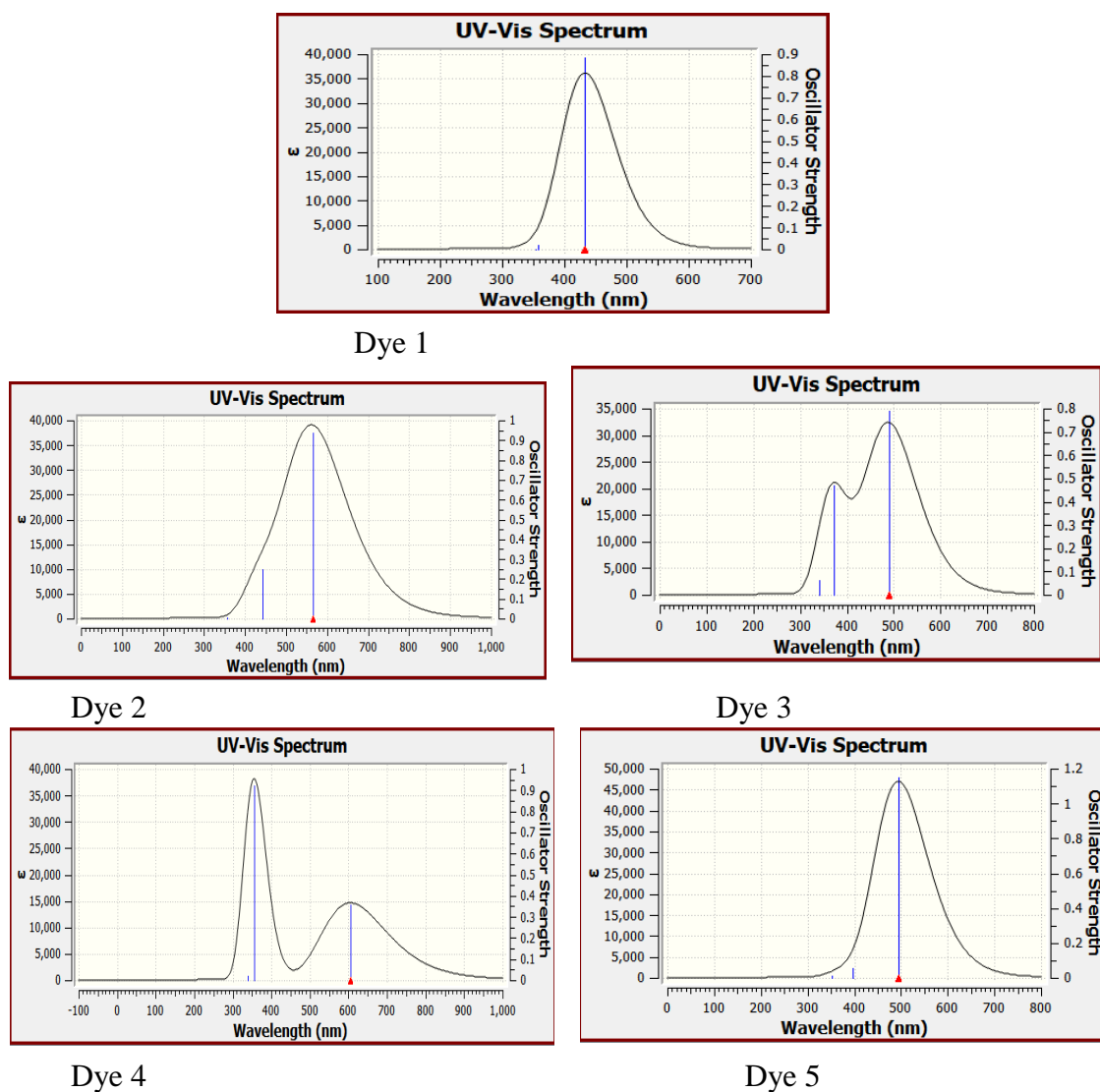


Figure 5. The UV-Vis spectrums of dyes between wavelength (nm) and molar absorptivity (ϵ)

Table 2. The measurement results of electronic transitions on dyes 1-5

Dyes	Excitation States	E (eV)	E_{ks}	$\lambda_{(eks)}(nm)$	The configuration of molecular orbital	f
1	1	2.9526	433.5577	HOMO-1 \rightarrow LUMO (14,6655 %) HOMO \rightarrow LUMO (99,3621 %) LUMO \rightarrow HOMO (17,0711 %)	0.8869	
	2	3.5339	357.1054	HOMO-1 \rightarrow LUMO (95,3953 %) HOMO \rightarrow LUMO+1 (21,1342 %)	0.0212	
	3	3.5617	354.7890	HOMO-2 \rightarrow LUMO (95,9596 %) HOMO-2 \rightarrow LUMO+1 (25,6795 %)	1.4x 10 ⁻⁰⁵	
	1	2.1829	566.0112	HOMO \rightarrow LUMO (100,2164 %) LUMO \rightarrow HOMO (18,0469 %)	0.9359	
	2	2.7887	443.5726	HOMO-1 \rightarrow LUMO (40,4045%) HOMO \rightarrow LUMO (0.10940) (15,4716%) HOMO \rightarrow LUMO+1 (89,9123 %)	0.2493	
	3	3.4763	356.32828	HOMO-2 \rightarrow LUMO (40,2546 %) HOMO-1 \rightarrow LUMO (77,8348 %) HOMO \rightarrow LUMO+1 (32,6785 %) HOMO \rightarrow LUMO+2 (31,4764 %)	0.0029	
3	1	2.5882	604.8094	HOMO \rightarrow LUMO (99,5743 %)	0.3592	
	2	3.6321	355.6995	HOMO-1 \rightarrow LUMO (43,3969 %) HOMO \rightarrow LUMO+1 (87,7061 %)	0.9235	
	3	3.9218	338.7231	HOMO-4 \rightarrow LUMO (25,4971 %) HOMO-3 \rightarrow LUMO (15,0417 %) HOMO-2 \rightarrow LUMO (15,7007 %) HOMO-1 \rightarrow LUMO (71,6518 %) HOMO \rightarrow LUMO+1 (29,5884 %) HOMO \rightarrow LUMO+2 (50,2234 %)	0.0215	
	1	2.5260	489.9719	HOMO \rightarrow LUMO (99,4526 %)	0.7883	
	2	3.3313	372.8839	HOMO-1 \rightarrow LUMO (51,3124 %) HOMO \rightarrow LUMO+1 (83,8268 %)	0.4683	
	3	3.6388	341.7035	HOMO-2 \rightarrow LUMO (52,1148 %) HOMO-1 \rightarrow LUMO (73,0094 %) HOMO \rightarrow LUMO+1 (38,3142 %) HOMO \rightarrow LUMO+2 (15,3867 %)	0.0626	
5	1	2,5034	494.8777	HOMO \rightarrow LUMO (100,511%) LUMO \rightarrow HOMO (15,6131 %)	1,1529	
	2	3.1319	395.7559	HOMO-1 \rightarrow LUMO (47,7372 %) HOMO \rightarrow LUMO+1 (85,4914 %)	0.0537	
	3	3.5310	351.0817	HOMO-3 \rightarrow LUMO (17,4996 %) HOMO-2 \rightarrow LUMO (45,6767 %) HOMO-1 \rightarrow LUMO (77,2578 %)	0.0134	

The data in Figure 5 and Table 2 show that the dye 3 is better in absorbing light with the maximum spectral peak of maximum light absorption on 606.8094 nm wavelength and of the spectrum, it can be seen that the light absorption reaches the area of infrared (IR). If the molecules are capable of absorbing IR ray, thus, the molecules also capable of absorbing the UV- visible light. UV light has a higher light intensity and can be produced most optimally during 11 to 1 am [19]. The visible light is produced during the day light, while the dominant IR ray is produced during the evening. It means that the DSSCs instrument with dye 4 as the sensitizer is capable of absorbing light during the day or night time. It can be seen in Table 2 that in general the absorption peak is dominated by the presence of electronic transitions from HOMO \rightarrow LUMO exists in HOMO and LUMO contours that show the electronic transition from π to π^* . According to the f values, the LHE (Light Harvesting Efficiency) values can be known, in which (f) is the oscillator strength during the occurrence of electronic excitation on certain wavelengths. Oscillator strength is parallel with LHE, a higher oscillator strength acquired during the excitation will make the LHE value to be higher as well. A high LHE will produce a high electrical current.

3.4 The effect of adding electron withdrawing and donating groups

Dye 6 was determined as the optimal dye structure with the addition of electron withdrawing and donating groups.

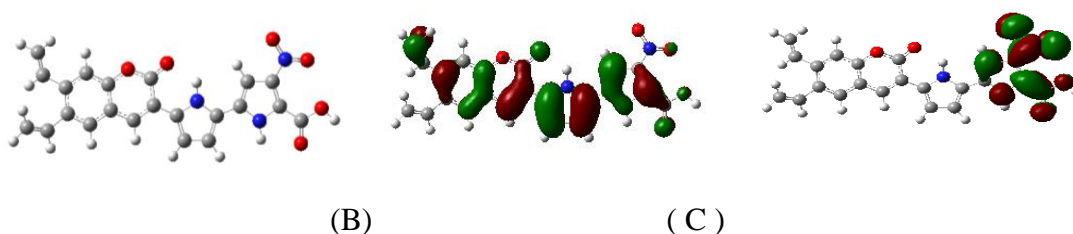


Figure 6. Optimal geometric structure (A), HOMO contour (B), LUMO contour (C) of dye 6

Of the HOMO contour in Figure 6, it can be seen that the groups of $-C_2H_3$, Donor, and π chain are the groups contributing on donating electrons and the LUMO contour shows that the groups of NO_2 and formic acid are contributing as the acceptor of electrons.

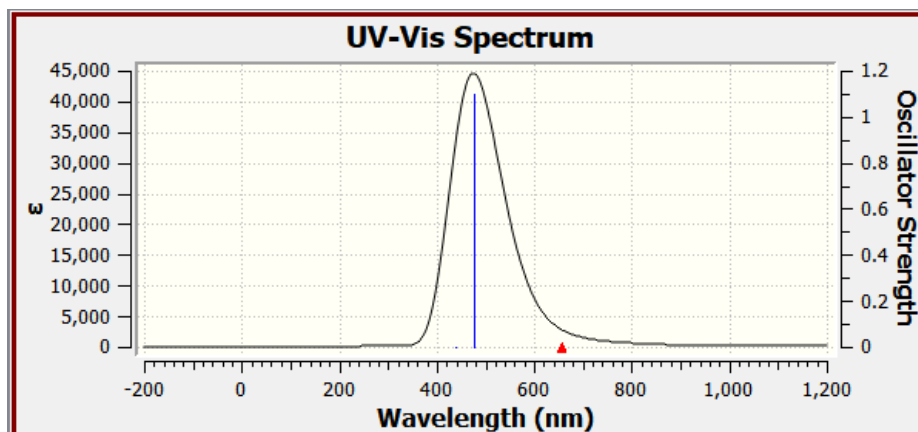


Figure 7. The adsorption spectrum of dye 6

Table 3. The electronic transition of dye 6

Dye	Excitation States	Excitation Energies (eV)	$\lambda_{\text{eks}}(\text{nm})$	The configuration of OM	f
6	1	1.8873	657.75	HOMO → LUMO (99,5998 %)	0.022
			35		8
	2	2.6057	475.30	HOMO → LUMO+1 (99,5192 %)	1.096
			56		4
	3	2.8332	438.44	HOMO-10 → LUMO (14,2696 %)	0.001
			15		9
				HOMO-6 → LUMO (16,8717 %)	
				HOMO-5 → LUMO (16,8717 %)	
				HOMO-3 → LUMO (35,4405 %)	

Dye 6 produced -5,4681 eV of E_{HOMO} and 3,1914 eV of E_{LUMO} values, therefore, 2,2767 eV ΔE was produced. It can be known that the addition of withdrawing and donating groups of electron decreased the band gap and increased the λ_{eks} of dye 3. The presence of $-\text{C}_2\text{H}_3$ group caused a longer resonance of π electrons and the presence of NO_2 group caused stronger withdrawing of electrons, therefore, the resonance of π electrons from the donor band to the acceptor to be easier. Longer and stronger resonance of π electrons caused the occurrence of red shift.

3.5. Electrical Properties

The electrical properties of DSSCs were discovered from the V_{oc} value (open current voltage), J_{sc} (current density), and power efficiency (η). The LHE and V_{oc} values can be seen in Table 4.

Table 4. LHE and V_{oc} values of dyes 1-6

Dyes	f	LHE	V_{oc}
1	0.8869	0.8702	0.8027
2	0.9359	0.8841	1.1251
3	0.9235	0.8807	1.3012
4	0.7883	0.8372	1.1575
5	1.1529	0.9297	0.9387
6	1.0964	0.9199	0.8086

According to the formulation, it can be known that a greater LHE will make a greater current density (J_{sc}) and the highest of J_{sc} and V_{oc} will make the power efficiency to be greater as well [24]. According to the LHE values, dye 5 produced greater power efficiency. However, according to the V_{oc} value, dye 3 produced greater power efficiency.

4. Conclusion

Dye 3 with coumarin-3-dipyrrole-2-carboxylic acid structure had longer wavelength between the chain variations of π -conjugation in which the light absorption of dye 3 reached the infrared area. The addition of C_2H_3 donating group or $-NO_2$ withdrawing group can decrease the band gap. Therefore, it can be concluded that dye 3 was the most efficient as the sensitizer on DSSCs instruments and the addition of electron withdrawing and donating groups on dye 3 can improve the light absorption efficiency of dyes.

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