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Theoretical Study of The Structure of Anthocyanin Dyes to Improve The Performance of Dye Sensitized Solar Cells (DSSCs)

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Abstract

In this study, anthocyanin dyes have been designed in two ways: without modification and with modification, incorporating donor chains and π-chains, and forming the structure of type D-π-A dyes. The anthocyanin dyes used are delphinidine, cyanidin, pelargonidin, malvidin, petunidine, and fragarine. Meanwhile, the modified molecule is a combination of anthocyanin dye as an acceptor chain, coumarin as a donor chain, and 1,4-dihydro-pyrrolo[3,2-b]pyrrole as a π-conjugation chain. The molecular structure was calculated using a 16W Gaussian Software with the DFT method and the B3LYP/6-31G base set. The results of the calculation on the dye without modification showed that the malvidin dye produced the smallest bandgap of 2.4085 eV and the largest light absorption. Meanwhile, the results of the calculation of the modified dye showed that the modified dye with the delphinidin acceptor produced the smallest bandgap of 1.4485 eV and the largest light absorption. In conclusion, modified anthocyanin dyes can improve the light absorption efficiency in DSSCs.

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INTRODUCTION

Energy has an important role in aspects of human life. Currently, energy sources still depend on fossil fuels. With fossil fuel reserves decreasing, countries around the world are trying to develop alternative renewable energy sources (Hardeli et al. 2013). Of the various available energy sources, solar energy is one of the alternative energy sources that has great potential to be developed but has not been utilized optimally (Nurhidayah et al. 2018). Utilizing solar energy sources is an effective way to overcome the current energy crisis with advantages such as being abundant and not causing greenhouse gas emissions or other pollutants (Li et al. 2019).

Solar cell equipment (photovoltaic) is able to convert sunlight into electrical energy(Imelda 2017). There are several types of solar cells, one of which is Dye Sensitized Solar Cells (DSSCs) which is an interesting research topic and is widely carried out because the manufacturing process is simple, relatively cheap, and environmentally friendly(Li et al. 2019). Sensitizers are one of the most important components in DSSCs equipment that plays a role in absorbing light that will be converted into electrical energy (Chaiamornnugool et al. 2017).

The sensitizers used in DSSCs are derived from organic dyes and metal complexes. Although sensitizers of ruthenium metal complex compounds produce relatively high efficiency, they have not been mass-produced due to the limited availability of metals, high manufacturing costs, complex synthesis processes, and difficulty in degradation. To overcome this, organic compounds can be used as sensitizers which are an alternative way to reduce the cost of solar cell production and are expected to replace the sensitizer of ruthenium dye (Chaiamornnugool et al. 2017).

Anthocyanins are one of the organic compounds that belong to the flavonoid group, found in plant parts such as fruits, leaves, stems and flowers. Anthocyanins have hydroxyl groups and conjugated π bonds so that they act as electron acceptors and can bind to TiO2 semiconductors in DSSCs. However, in general, organic compounds have disadvantages such as low stability and light absorption efficiency, so a modification of the dye is required.

D-π-A type dye (Donor-π-conjugated-Acceptor) is a type that is widely analyzed as a sensitizer in DSSCs using a computational program with the Density Functional Theory (DFT) calculation method which has the advantage of being more accurate calculation results (Pranowo 2016). In addition, dyes with type D-π-A have good stability and efficiency in DSSCs because they have push and pull properties (Pramanik et al. 2015). Therefore, the author is interested in carrying out a study, namely to theoretically compare unmodified anthocyanin dyes with anthocyanin dyes that are modified to form a D-π-A type structure using the DFT calculation method.

METHOD

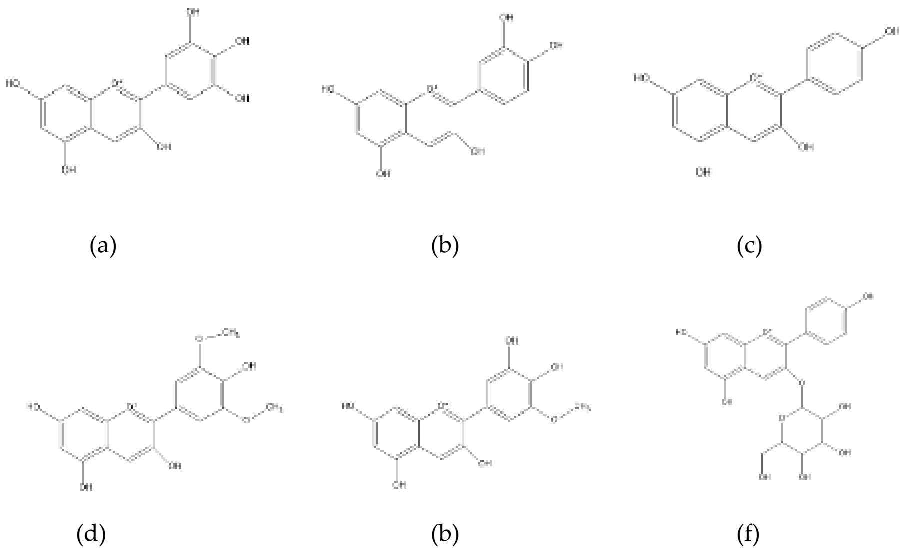
Equipment

In this study, the equipment used is a laptop with an Intel (R) Core (TM) i3-5005U processor @ 2.00 GHz 2.00 GHz, 8.00 GB RAM and a 16W Gaussian Software.

Drawing and Optimization, Structure of Anthocyanin Dyes Without Modification and Modified

The molecular structure of each dye is described using GaussView 6.0.16 and the optimization process takes place at Gaussian' 16W with the base set B3LYP/6-31G. In this study, molecular modeling of anthocyanin dyes was carried out without modification and with modifications to form a D-π-A type structure to determine molecules that have the potential to be sensitizers in DSSCs. The structure of the anthocyanin dye used can be seen in Figure 1.

In modified anthocyanin dyes, the donor chain used is coumarin and the π-conjugation chain is 1,4-dihydro-pyrrolo[3,2-b]pyrrole. While anthocyanins act as acceptor chains. Modified dyes with acceptor chains of delphinidin, cyanidin, pelargonidin, malvidin, petunidine and fragarine are then referred to as dyes A, B, C, D, E and F respectively.



(a) (b) (c)

(d) (b) (f)

Figure 1. Molecular Structure of Anthocyanins (a) Delphinidin (b) Cyanidine (c) Pelargonidin (d) Malvidin (e) Petunidin (f) Fragarin

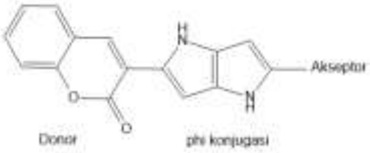
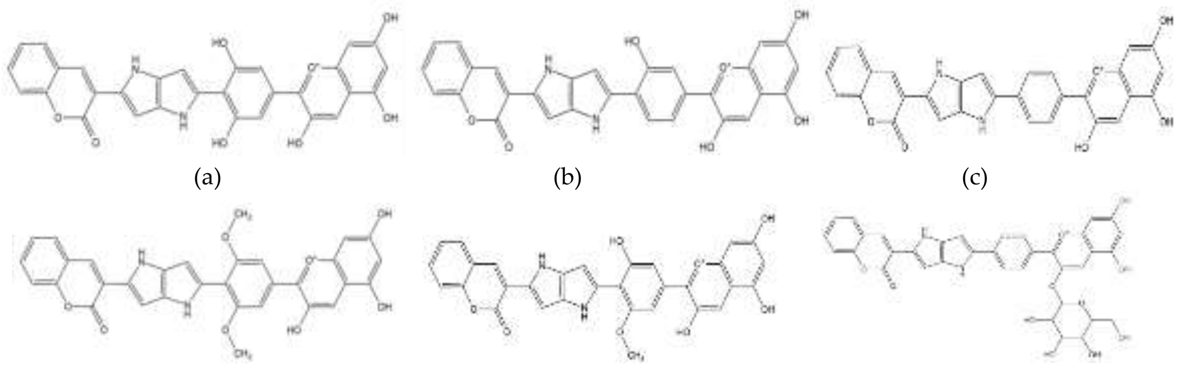


Figure 2. Molecular Structure of Dye Type D-π-A



(a) (b) (c)

(d) (e) (f)

Figure 3. Molecular Structure of Dye Type D-π-A Acceptor Chain Variation (a) *Dye* A (b) *Dye* B (c) *Dye* C (d) *Dye* D (e) *Dye* E (f) *Dye* F

External Data Reading Process

The optimized color substances are stored in the form of 3 files, namely gjf for initial depiction, chk depiction after optimization and notepad. The data output can be read based on the saved notepad and then analysis is carried out in the form of:

1. Electronic parameters are HOMO and LUMO contours, EHOMO, elumo, bandgap (ΔE), and dipole moment
2. Optical parameters are absorption spectrum, excitation wavelength (λexcitation), Light Harvesting Efficiency (LHE), and oscillator strength (f)
3. The electrical parameters are open current voltage (VOC), current density (JSC) and energy conversion efficiency (η)

Some of the equations used are:

$\Delta E = E_{LUMO} - E_{HOMO}$ (1)

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

$JSC = \int LHE(\lambda)\Phi_{inject}\,\eta_{collect}\,d\,l$ (3)

$VOC = E_{LUMO} - E_{CB}$ (4)

the $= JSC\ V_{OC}\ (Ff)\ /Is$ (5)

FF = *Fill factor*

Is = Light intensity

Φinject = Electron injection efficiency

ηcollect = Electron collection efficiency

ECB (energi pita konduksi TiO2) = -4,0 eV

Based on these parameters, an analysis of the efficiency of dyes as sensitizers in DSSCs was then carried out (Wang et al. 2018).

RESULTS AND DISCUSSION

Optimal Geometric Structure of Anthocyanin Dyes Without Modification

The geometric structure of anthocyanin molecules has been optimized using the B3LYP/6-31G set base. Optimization is carried out to obtain optimal molecular structure. From the optimal structure, the electronic properties can be determined, namely HOMO energy, LUMO energy, bandgap, and HOMO-LUMO contour of each dye. The contour of HOMO-LUMO consists of the HOMO band being an electron donor while the LUMO band is an electron acceptor(Imelda et al. 2020). Anthocyanin dyes without modification obtained the most efficient results, namely in malvidin dyes. The optimal geometric structure and contour of the anthocyanin dye HOMO-LUMO is shown in Figure 4.

Based on Figure 5, it is known that overall the contour of HOMO is on the aromatic chain C6 and the contour of LUMO is on the aromatic chain C6-C3 so that it can be concluded that the C6 chain is an electron donor and the C6-C3 chain is an electron acceptor. So that when the dye molecule is exposed to light, there will be electron transfer from the C6 chain to the C6-C3 chain.

Bandgap and Dipole Moment of Anthocyanin Dye Without Modification

The bandgap value determines whether or not the electron is easily excited from the HOMO band to the LUMO band. Based on Planck's Law, which is E = h.c/λ, the smaller the ΔE, the light will be absorbed at a larger wavelength, where the greater the wavelength, the more light will be absorbed. This is due to the easier process of electron excitation from low-energy orbitals (HOMO) to high-energy orbitals (LUMO), so that the sensitivity to light is also increasing(Imelda et al. 2020). From Table 1, it can be seen that the malvidin dye has the smallest bandgap of 2.4085 eV which has the best light absorption efficiency. The low bandgap value in malvidin is due to the aromatic chain C6 there are 2 -OCH3 groups which will reduce the impulse of the positive mesomeri effect of the hydroxyl group so as not to block the electron resonance path. The easier the electron resonance, the light will be absorbed at a longer wavelength (red shift). The dipole moment of the anthocyanin dye without modification is listed in Table 1. From the data, it is known that malvidin has the largest dipole moment, while pelargonidin has the smallest dipole moment. This is due to the malvidin presence of the -OCH3 group as the driving group that can facilitate the transfer of electrons from the C6 chain to the C6-C3 chain.

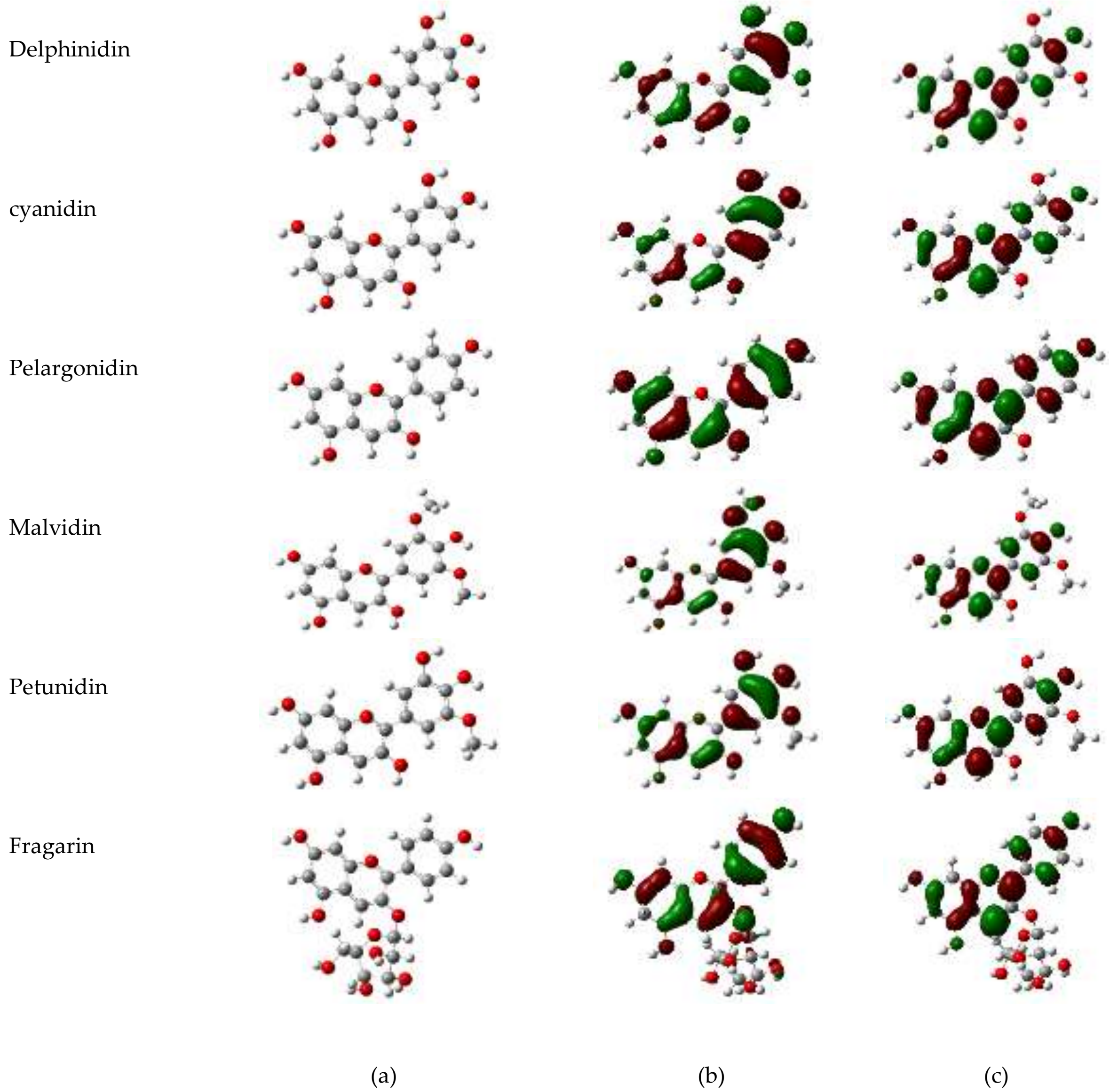


Figure 4.Struktur Geometri (colour of atom C= grey, O= red, H= white) (a) *contour* HOMO (b) dan *contour* LUMO (c) of Dyes Delphinidin, Cyanidin, Pelargonidin, Malvidin, Petunidine and Fragarine

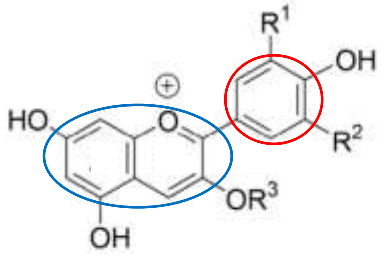


Figure 5. C6-C3 (blue circle) and C6 (red circle) Chains on Anthocyanins

Table 1. The Results of The Calculation of HOMO Energy, LUMO Energy, Bandgap (ΔE), and The Dipole Moment Anthocyanin Dye Without Modification

Dye	E_{HOMO}(eV)	E_{LUMO}(eV)	ΔE(eV)	Momen Dipol (Debye)
Delphinidin	-9.0317	-6.4872	2.5445	8.006104
cyanidin	-9.0570	-6.4758	2.5812	6.091411
Pelargonidin	-9.2658	-6.4752	2.7906	5.366492
Malvidin	**-8.7251**	**-6.3166**	**2.4085**	**8.281985**
Petunidin	-8.9204	-6.4064	2.5140	8.118644
Fragarin	-8.8777	-5.9756	2.9021	6.205310

Spectrum of Absorption of Anthocyanin Dyes Without Modification

In Figure 6. It is known that the dye pelargonidine has the greatest molar absorpivity shown from the highest absorption peak than other anthocyanin dyes. Meanwhile, malvidin dyes produce absorption at longer wavelengths which is characterized by a wider absorption peak than other anthocyanin dyes. Efficient dyes should produce high and wide absorption peaks. However, wavelength has more effect on the efficiency of light absorption. So based on the UV-Vis spectrum, it is known that the most efficient dye is malvidin dye.

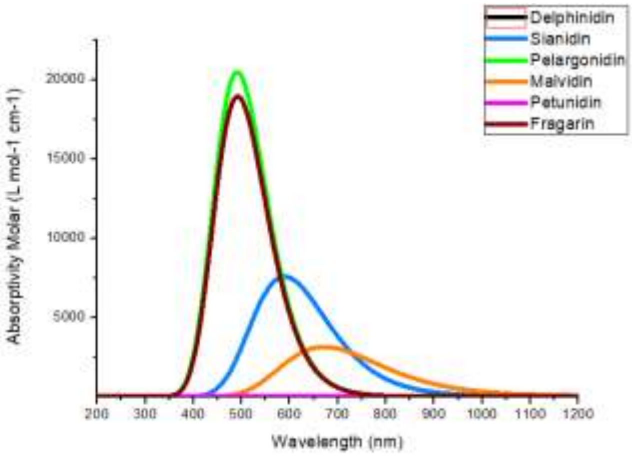


Figure 6. UV-Vis Spectrum of Dyes Delphinidin, Cyanidin, Pelargonidin, Malvidin, Petunidine, and Fragarine between Wavelengths (nm) with Absorptivity Molar (ε)

The data in Figure 6. and Table 2. show that malvidin dyes are able to absorb light up to the near Infrared Red (IR) region which has an absorption shift up to a wavelength of 1050.62 nm, the lowest excitation energy is 1.0075 eV, and the electron transition from the HOMO to LUMO band is produced as shown in the Molecular Orbital (OM) configuration section table. If the molecule is able to absorb IR rays, the molecule is also able to absorb Ultra Violet (UV) rays as well as visible rays.

At 11.00-13.00 UV rays produce a greater and most optimal light intensity. Visible rays are produced during the day and dominant IR rays are produced at night(Imelda et al. 2020). DSSCs equipment with malvidin dye sensitizers are able to absorb light during the day and at night. Therefore, it is known that dyes are efficiently used as sensitizers in DSSCs, namely they can absorb most of the solar radiation in visible and near-IR areas, and can produce a large photocurrent response(Sanusi et al. 2019).

The intensity of the transition can be expressed in the form of oscillator strength (f) which is directly related to the wave function from the initial to the end of the transition state (W 1996). So that the value of light absorption efficiency (LHE) can be determined from the value f produced, where f is the oscillating force when electron excitation occurs at a certain wavelength. Oscillator strength is directly proportional to LHE, that is, the greater the oscillator strength, the greater the LHE value obtained. The greater the LHE value, the more light will be absorbed(Obotowo, Obot, and Ekpe 2016).

Table 2. Results of the calculation of the electronic transition of anthocyanin dyes without modification

Dye	λexcitation (nm)	Excitation energy (eV)	OM Configuration	*f*
Delphinidin	866.63	1.4306	H→L = 99.40%	0.0002
	665.20	1.8639	H-1→L = 98.00%	0.0129
	577.03	2.1487	H-2→L = 97.48%	0.0527
cyanidin	942.00	1.4725	H→L = 98.75%	0.0022
	625.36	1.9826	H-1→L = 97.34%	0.0004
	498.27	2.4883	H-2→L = 97.54%	0.0104
Pelargonidin	838.87	1.4780	H→L = 99.63%	0.0506
	546.51	2.2686	H-1→L = 97.91%	0.0362

Dye	λexcitation (nm)	Excitation energy (eV)	OM Configuration	*f*
	487.39	2.5438	H→L = 92.66%	0.4906
			H-1→L = 37.92%	
Malvidin	1050.62	1.0075	H→L = 99.98%	0.0773
	764.55	1.6217	H-1→L = 97.62%	0.0434
	672.73	1.8430	H→L = 78.84%	0,0774
			H-1→L = 61.74%	
Petunidin	857.87	1.1720	H→L = 15.96%	3.81 x 10-5
	701.62	1.7671	H-1→L = 98.12%	0.0000
	607.21	2.0419	H-2→L = 97.61%	0.0006
Fragarin	848.73	1.4608	H→L = 99.38%	0.0469
	517.38	2.3964	H→L+1 = 14.74%	0.0326
			H-1→L = 25.52%	
	486,64	2.5478	H-2→L = 93.98%	
			H→L = 96.38%	0.4625
			H-2→L = 24.56%	

Analysis of the Electrical Properties of Anthocyanin Dyes

The ability of a dye as a sensitizer in converting solar energy into electrical energy can be reviewed from electrical parameters in the form of VOC, JSC, and η values. Based on equation (5) it is known that η will increase if the VOC and JSC increase. The LHE value is directly proportional to the JSC and wavelength, so to get a high Jsc, the dye molecules used in DSSCs must have LHE and a large light wavelength (Obotowo, Obot, and Ekpe 2016; Seo et al. 2016).

Based on the data in Table 3, it was found that malvidin dyes produce greater LHE. The more light is absorbed by the dye molecules, the greater the oscillator strength produced and the LHE value will also be greater because based on equation (2) the oscillator strength is directly proportional to the LHE value. JSC is the density of current flowing in every 1 cm^2 of cells, based on equation (3) the value of JSC is influenced by the value of LHE and λ. The greater the value of LHE and λ, the greater the value of JSC. VOCs denote open current stress where stress is defined as the magnitude of the force exerted by molecules on the cross-sectional area. The longer the electron moves, the higher the voltage produced so that the greater the value of the VOC produced.

A negative VOC value indicates that electrons are transferred from low potential to high potential and that number can be absolute. So based on the absolute value, delphinidin produces the highest VOC value. The VOC value in delphinidin is greater than that of other anthocyanin dyes because delphinidin molecules tend to be more planar so electron transfer will be easier. Negative VOC values were also produced in the previous study, namely a study conducted by Abdel-Mottaleb et al in 2014. From the results of amphibiolic cyanide dye optimization, ELUMO was obtained at -6,070 eV, so that the VOC value was -2,070 eV(Abdel-Mottaleb et al. 2014). The efficiency of energy conversion is affected by the intensity of light. Based on equation (5) the energy conversion efficiency is inversely proportional to the intensity of light, so the smaller the light intensity, the greater the energy conversion efficiency produced. In addition, the larger the wavelength, the smaller the value of light intensity.

Optimal Geometric Structure of Modified Anthocyanin Dyes

Anthocyanin dyes modified with the addition of donor chains and π chains have been optimized using the B3LYP/6-31G base set. From the optimal structure, electronic properties can be determined, namely HOMO energy, LUMO energy, bandgap, HOMO-LUMO contour as well as optical properties such as absorption spectrum, excitation wavelength, LHE, and oscillator strength. The modified anthocyanin dye obtained the most efficient results on dye A. The optimal geometric structure and contour of the modified anthocyanin dye HOMO-LUMO are shown in Figure 7.

Based on Figure 7. in dye A, it is known that the delphinidin chain acts as an electron acceptor because in the contour of LUMO it can be seen that the density or the largest electron density is in the delphinidin chain. A good sensitizer, the electron density in the HOMO region is around the donor chain with an energy level lower than the energy level of the $I^-/I3^-$ electrolyte (-4.8 eV), so that when the dye is oxidized after the electrons are injected into the TiO2 conduction band it can be regenerated by the $I^-/I3^-$ electrolyte. In addition, the electron density in the LUMO region is around the acceptor chain with an energy level higher than the energy level of the TiO2 conduction band (-4.0 eV) which aims to facilitate the injection of electrons into the semiconductor(Obotowo, Obot, and Ekpe 2016). The contours of HOMO and LUMO show the characteristics of charge transfer in dyestuffs. From the HOMO contour, it is known that coumarin is an electron donor while from the LUMO contour it is known that delphinidin is an electron acceptor.

Table 3. LHE and VOC values of anthocyanin dyes

Dye	LHE	VOC (eV)
Delphinidin	0.0005	-2.4872
cyanidin	0.0051	-2.4758
Pelargonidin	0.1010	-2.4752
Malvidin	0.1630	-2.3166
Petunidin	0.0001	-2.4064
Fragarin	0.1024	-1.9756

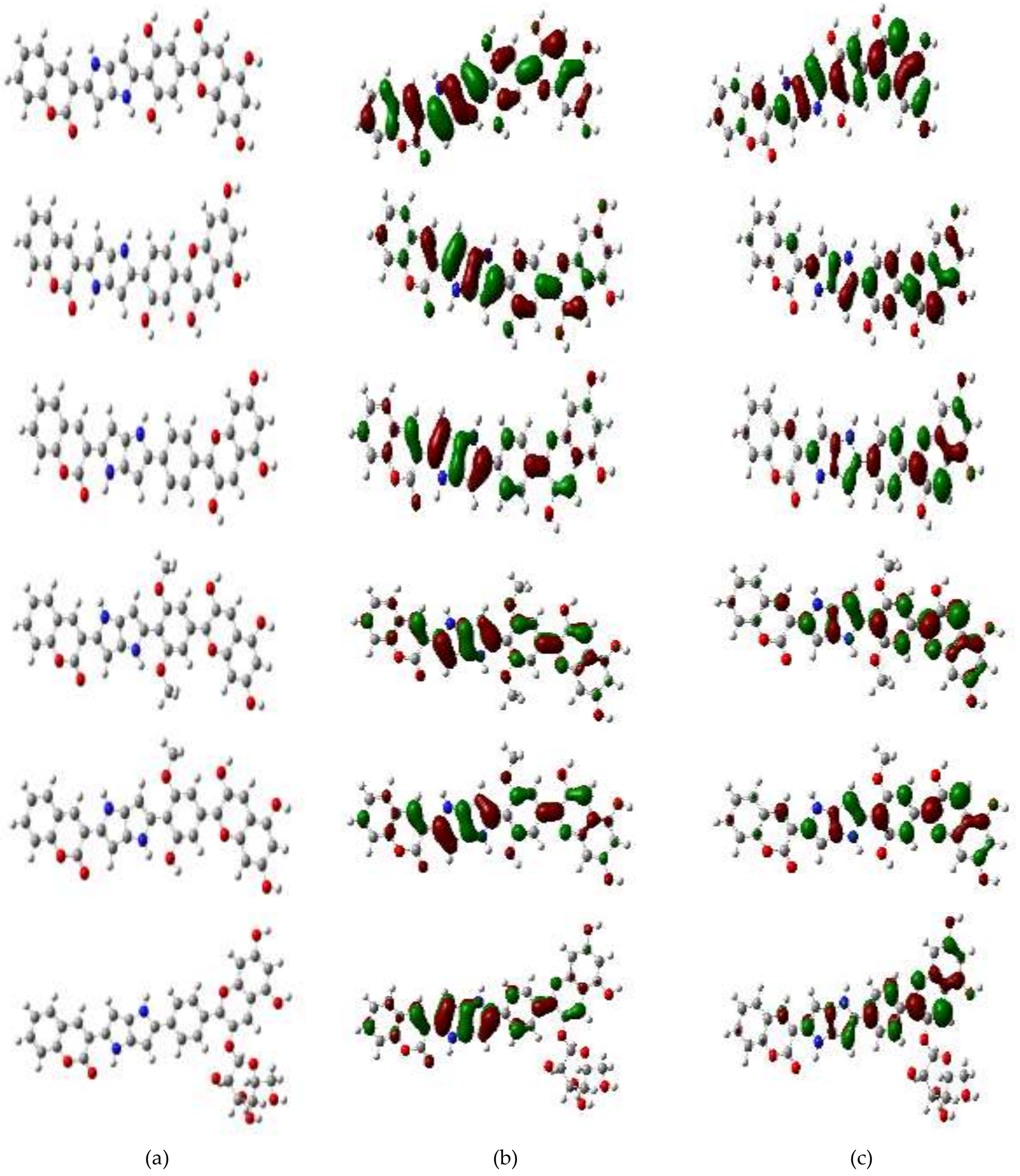

(a) (b) (c)

Figure 7. Geometric Structure (Atomic Color C = Gray, N = Blue, O= Red, H = White) (a) Contour HOMO (b) and Contour LUMO (c) of *Dye* A, *Dye* B, *Dye* C, *Dye* D, *Dye* E, and *Dye* F

Bandgap and Dipole Moment of Modified Anthocyanin Dye

The data in Table 4. show that the modified anthocyanin dye with a delphinidin acceptor chain (Dye A) has the smallest bandgap of 1.4485 eV which has the best light absorption efficiency. This is because delphinidin, which acts as an acceptor chain, has more -OH (hydroxyl) groups than other anthocyanin dyes. The -OH group attracts electrons, facilitating the resonance process of electrons π from the donor chain to the acceptor chain. The easier the resonance of electrons π the light will be absorbed at longer wavelengths. In addition, the more electron attractable groups in the acceptor chain will facilitate the process of electron injection into the TiO_2 conduction band (Chaiamornnugool et al. 2017).

The dipole moment of the modified anthocyanin dye is listed in Table 4.4. From this data, it is known that the largest dipole moment is found in Dye A, while the smallest dipole moment is found in Dye F. The larger the dipole moment, the easier it will be to transfer electrons from the donor to the acceptor.

Table 4. The Results of The Calculation of HOMO Energy, LUMO Energy, Bandgap (ΔE), and The Dipole Moment of The Modified Anthocyanin Dye

Dye	EHOMO(eV)	ELUMO(eV)	ΔE(eV)	Momen Dipol (Deybe)
***Dye* A**	**-7.1936**	**-5.7451**	**1.4485**	**16.403720**
Dye B	-7.2312	-5.7016	1.5296	14.634236
Dye C	-7.3106	-5.7214	1.5892	14.396966
Dye D	-7.1131	-5.6362	1.4769	15.661144
Dye E	-7.1546	-5.6948	1.4598	16.122744
Dye F	-7.0673	-5.4502	1.6171	13.620783

Spectrum Absorption of Modified Anthocyanin Dye

In Figure 8. it is known that anthocyanin dyes modified with delphinidin acceptor chains have the greatest *molar absorptivity* or molar absorption as shown from high absorption peaks and produce uptake at longer wavelengths. This shows that the modified dye produces a high absorption peak as well as absorption at longer wavelengths compared to the unmodified anthocyanin dye. So it is known that modified anthocyanin dyes are more efficient than unmodified anthocyanin dyes.

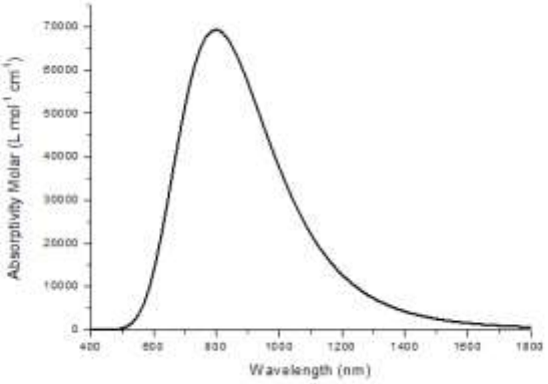


Figure 8. UV-Vis Spectrum of Modified Anthocyanin Dyes with Delphinidin Acceptor Chains between Wavelengths (nm) with *Absorptivity Molar (ε)*

Table 5. Results of electronic transition calculation of modified anthocyanin dyes

Dye	λexcitation (nm)	Excitation energy (eV)	OM Configuration		*f*
Dye A	1298.07	0.3983	H→L	= 97.34%	0.81100
	722.32	1.5535	H→L	= 35.81%	0.07136
	612.94	1.7165	H-1→L+1	= 31.81%	0.00000
			H-2→L+1	= 15.62%	

Based on Figure 8. and Table 5. It is known that delphinidin-based modified anthocyanin dyes are able to absorb light better which has an absorption shift up to a wavelength of 1298.07 nm with the lowest excitation energy of 0.3983 eV which is the transition of electrons from the HOMO to LUMO bands. This shows that modified anthocyanin dyes produce light absorption at longer wavelengths than unmodified anthocyanin dyes. Based on the calculation results, the LHE value was 0.8454 and the VOC value was 1.7451 eV. This dye also exhibits greater energy conversion efficiency. The increase in the value of light absorption efficiency in modified anthocyanin dyes is due to the effect of attraction and thrust on the molecule so that when exposed to light, there will be a longer resonance of π electrons from the donor band to the acceptor band. The greater the value of light absorption efficiency, the greater the energy conversion efficiency produced.

CONCLUSION

Based on the research that has been conducted, it can be concluded that anthocyanin dyes have been optimized in 2 ways, namely without modification and modification with the addition of donor chains and π chains so as to form the structure of dyes type D-π-A. The results of the calculation on the dye without modification showed that the malvidin dye produced the smallest bandgap of 2.4085 eV, light absorption of up to 1050.62 nm, the LHE value of 0.1630 and the VOC value of -2.3166 eV. Meanwhile, the results of the calculation on the modified dye showed that the modified dye with the delphinidin acceptor chain produced the smallest bandgap of 1.4485 eV, light absorption of up to 1298.07 nm, the LHE value of 0.8454 and the VOC value of 1.7451 eV. Based on the values of *bandgap*, λ, LHE, Voc, it is known that the modified dye shows better light absorption efficiency and energy conversion so that it can improve the performance of DSSCs.

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