



## Theoretical Study of Betalain Compounds from Binahong with a Red Trunk as DSSC (Dye-Sensitized Solar Cell) Material with the DFT (Density Functional Theory) Method

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**ABSTRACT:** Binahong with a red trunk is known to contain betalain which has the potential to be used as DSSC. Therefore, theoretical research was conducted on the potential content of betalain in binahong with a red trunk using computational methods. This research was conducted using density functional theory (DFT) with the B3LYP functional and with a base set of 6-311G(d). The band gap value of HOMO-LUMO was obtained as a reference for the effectiveness of binahong with a red trunk as a DSSC material. The results of this study indicate the band gap of betalain is 3.152685477 eV. The band gap shows how easy it is for betalain to excite electrons, from the band gap it can be concluded that betalain is a material that has a very high potential for effectiveness as a material for making DSSC.

**KEYWORDS:** Band Gap, Betalain, DSSC, HOMO, LUMO.

### INTRODUCTION

There is an intensification of the search for renewable energy resources now, due to the depletion of the supply of fossil energy resources such as crude oil [1]. One alternative of renewable energy resources is solar panels as a solar power plant or solar cell. However, the price of solar cells is not cheap, as well as some of the disadvantages of solar cells, such as the period of use which has a time limit. Solar cells also have a less effective level of light absorption, so the light has not been absorbed completely. From the solar cell itself, it has another form, namely the Dye-Sensitized Solar cell (DSSC).

Dye-Sensitized Solar Cell (DSSC) is a type of solar cell made using organic compounds. Before conducting direct research, which has a risk of human error, a theoretical study is carried out using computational methods. Computational methods also have a cost advantage when compared to research using direct experiments, the costs incurred from research using computational methods are much cheaper. If there is a discrepancy in the research material, the direct experimental method will require a fairly expensive cost to replace the failed material with new material. Unlike the case with computational methods where when there is a mismatch of materials and must use new materials, in computing there will be no cost at all because research and materials are obtained quite easily and do not require other costs.

From this, calculations are carried out using computational methods which have the aim of researchers being able to see the level of effectiveness of a material when it will be used for research. Where computational calculations have an error rate that is close to zero, because these calculations are not carried out by humans, but are carried out by computer systems.

In a theoretical study that uses this computational method, the process is carried out by mathematical calculations carried out by a computer to process a number-based simulation by the principles of making DSSC or Dye-Sensitized Solar Cell, which is a solar power plant that has the concept of electron transfer or electron cycle of the working electrode and the counter electrode. In this DSSC concept, several dyes can be used, one of which is natural dyes which are very abundant in Binahong with red stems. Namely Betalain.[2] Binahong is a very abundant plant in Asia, so it is not difficult to find it. Binahong with the scientific name *Anredera Cordifolia* is a medicinal plant that has many benefits, especially in the medical field. Binahong whose stems are red also has a lot of betalain content so it has a high enough potential when used as an ingredient for making Dye-Sensitized Solar Cells.[3]

Researchers chose Binahong with a red trunk because in previous studies betalain was found in Binahong with a red trunk, this was also reinforced by research by Pawar which stated that the red color contained in betalain was a result of betalain contained in binahong with a red trunk.[4][5] Betalains are easily soluble in nitrogen-containing water. Betalain itself is a compound that has a purple-red and yellow color, which is a compound with an excellent electron donor.



This research was conducted using the DFT (Density Functional Theory) method with B3LYP and base set 6311G(d). DFT is used because when compared to other methods, this method has a high level of accuracy or has the most similar results to the experimental results. The DFT method works by only solving the Schrodinger equation, this is because the DFT method works based on the level of electron density. [6]

Also used functional B3LYP was chosen because it can process the prediction of the properties and electronics of the compound. B3LYP itself is an approach to DFT exchange-correlation that works by incorporating the exact exchange portion of HF with correlation exchanges from other (experimental) sources.

The basis set 6-311G(d) is used because this basis has results that are by experimental results. With this method, the energy will be determined based on the value of the gap between the HOMO and LUMO values obtained from calculations performed with the NwChem application.

In this study, researchers will examine the band gap value of the betalain compound HOMO-LUMO using a computational method so that it can be used as a reference in the experiment of making Dye-Sensitized Solar Cells using Binahong with red stem material.

## METHODS

### Material

The research was conducted with the Microsoft Windows 10 Pro operating system with build version 10.0.18363; 18363, AMD Ryzen 3 2200U processor; 128 Gb SSD; VGA Card AMD Radeon™ Vega 3 Graphics; 4.00 Gb of RAM and also a Linux-based operating system using ubuntu with version 20.04.1-desktop version build which is accessed with the help of the virtual-box application. The applications used are Chem sketch, Avogadro, NwChem, and Terminal or Command Prompt. The dam uses the betalain structure to determine the band gap.

### Procedure

#### Initial Modeling

The molecular structure of betalain was drawn using Chem sketch and saved in MDL molfiles file format. Although what is needed in the running process is data from a 3D structure image, in this process the compound is only drawn in 2D, and in a simple form, so even though the shape is not so perfect, it will optimize energy so that the compound is in the most perfect form. Because this 2D structure will be automatically converted into a 3D structure in the Avogadro application in the Optimize Geometry stage

#### Optimize Geometry

The file format MDL molfiles is entered into the Avogadro application. In this process, the 2D structure that was drawn will be automatically converted into a 3D structure. Then optimize geometry is done, so that when the process is running, the data from the betalain structure is in a stable state, and the description is replaced on the "preview" menu, where the text that says "SCF" or "self-confidence field" is replaced with "DFT" or "Density Functional Theory", with a very high level of accuracy in computational modeling.

Then the file is saved in a file format (.nw), with the aim that the file is read by the NwChem application, because in determining the band gap, in this study the NwChem application was used.

#### Determination of the Band Gap

Then, before running with the NwChem application, the file is transferred from the Microsoft Windows operating system to the Ubuntu operating system using Google Drive. This is because files from the Microsoft Windows operating system cannot be directly transferred to the Ubuntu operating system, so an intermediary is needed. One way that can be used is to upload files from the Microsoft Windows operating system to Google Drive, then download them from Google Drive using the Ubuntu operating system.

On the Ubuntu operating system, files are placed in specific folders that are not filled with other files. This is done to avoid bugs when running the process.

The folder that was created earlier, is opened using a terminal application or a command prompt, then the files in the folder are checked, to ensure that the files have been read. Then the file is entered into the application using the command on the terminal, and the running command is performed.

In the folder, the results of running will be automatically saved in a file format (.log). The file cannot be directly accessed on the Ubuntu operating system but must be moved back into the Microsoft Windows operating system. At the time after being moved to the Microsoft Windows operating system, the file will automatically be read as a note file in the format (.txt).

## RESULTS

### Initial Modeling

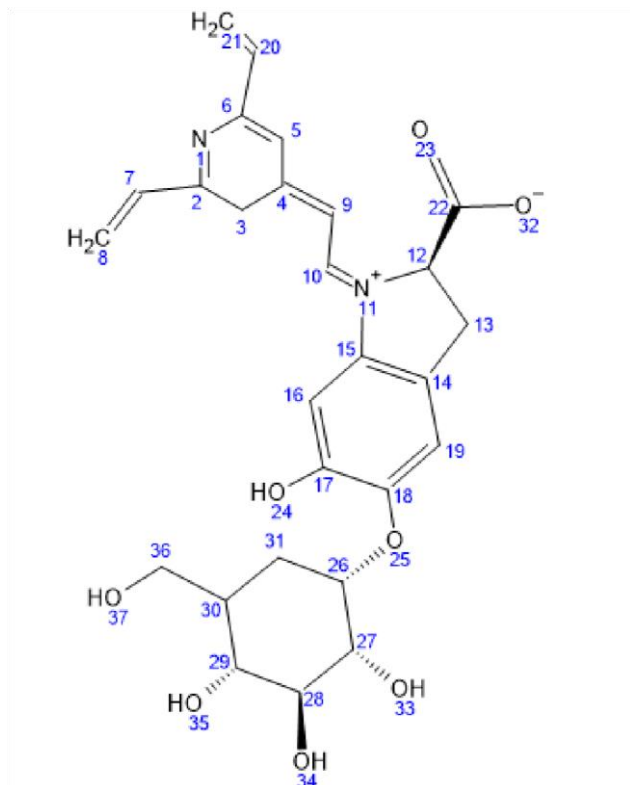


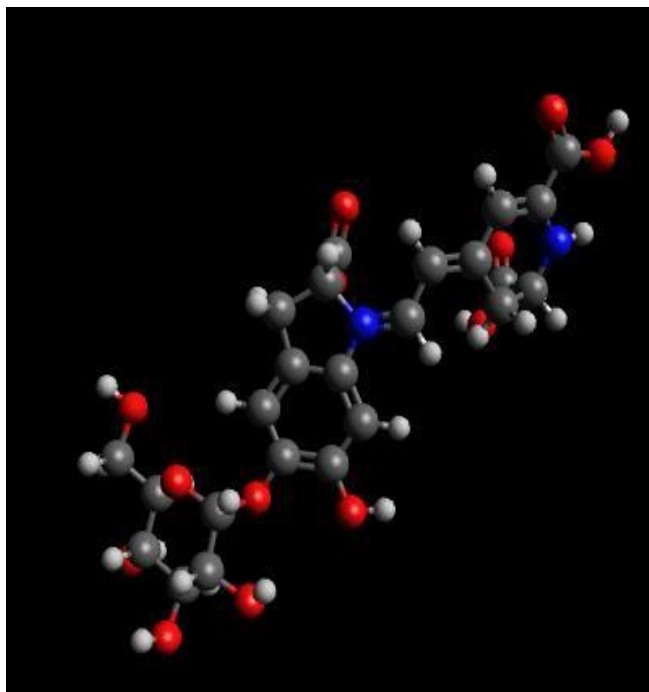
Figure 1. Visualization of 2D Betalain Structures using Chem sketch

First of all the file is drawn with the Chem sketch application. In this research, 2D and 3D molecular structures are needed. The 2D Betalain structure was drawn using the Chem sketch application. The structure of betalain with the molecular formula  $C_{24}H_{26}N_2O_{13}$  was drawn using the Chem sketch chemical application, then saved in a file format MDL molfiles so that it can be processed using the Avogadro application.

In this process, there is no need to draw a Betalain 3D Structure because the Structure will be automatically created in the Avogadro application. So, in the process of making the initial model, only the Betalain Structure is needed in the form of a 2D structure.

### Optimize Geometry

Files with the format MDL molfiles are entered into the Avogadro application and will be immediately converted into the 3D form so that they can be processed by the next program. Then optimized geometry is done from the extension menu, in this process, the system will optimize the geometric shape of the 3D structure from betalain compounds to the most optimal shape. Then the NwChem menu is selected in the extension menu, this is done because in determining the HOMOLUMO value as an ingredient to find the band gap value, the next file will be processed using the NwChem application on the Ubuntu operating system.[2]



**Figure 2.** Visualization of the Betalain 3D Structure after being optimized using Avogadro

In the setting option, a Single Point Energy (SPE) calculation is used with the B3LYP theory or hybrid functional and is carried out with a 6-311G(d) basis set, because the B3LYP method and the 6-311G(d) basis set have results that are by experimental results, this is also reinforced by research by Sudarlin who found the results of 89.39% similarity between experiments using the Harborne method and computational calculations with the theory of B2LYP basis set 6-311G(d).[7]

This level of dissimilarity of 10.61% is unlikely if it is caused by an error in the system in carrying out calculations, this can occur with the assumption that errors or inaccuracies in the results are caused by external causes, both impurities in the binahong extract sample when conducting experiments or as a result from the researchers themselves, so there was a data discrepancy even though it was very small. This assumption is based on almost absolute computations with computational methods, because it is known that the computational method uses calculations performed by computer systems and is not calculated directly by humans, so the level of possibility of errors in calculations is 0 or it can be said to be very impossible.[8]

Then the description is replaced on the "preview" menu, in the text that says "SCF" or "self-confidence field" it is replaced with "DFT" or "Density Functional Theory", this method was chosen because it has a very high level of accuracy in computational modeling. Then select the generate option to generate the final file that is ready to run. By selecting the generate option, you will be directed to save the file with the file format (.nw) which means it is ready to run with the NwChem application.

### **Determination of the Band Gap**

Files are transferred from Microsoft Windows to Ubuntu by uploading them to Google Drive via Microsoft Windows and then downloading them from Google Drive in Ubuntu. This is done because even though on the same computer, these two operations cannot be combined between the storage, so they cannot directly transfer files from Microsoft Windows to Ubuntu and are required to use the help of other methods such as moving files with the help of Google Drive or other methods. which allow.

Then the downloaded file is put into a specific folder so that no bugs occur when processed using the terminal or commonly called the command prompt. The folder that has been created is opened in the terminal with the command (`cd /"folder"`). This command is done to open the folder that contains the initial file to be run with the NwChem application. Then to check whether the file is read by the system, the command (`ls`) is executed. This command is intended to create a list of any files that are in the destination folder, with this command it will be shown whether the file is read or not. Files are entered into the NwChem application using the command (`NwChem "filename" > "filename".log&`). Then the running process is carried out with the command (`tail -f "file name that has been changed"`), this command intends to run the file that has been entered into the NwChem application. With



this command, the running process will take a relatively long time, this depends on the speed of the device used to carry out the running process.

The results will be directly saved in the previous folder with a file format (.log). This data file cannot be directly opened through the Ubuntu operating system, but must first be moved back into the Microsoft Windows operating system using the same method (via Google Drive).

Files that have been transferred to the Microsoft Windows operating system will automatically be read as notes in the (.txt) format. From the calculation data, the results are obtained as in the table. The result of HOMO is -0.206058 and LUMO energy is -0.090199.

**Table 1.** Betalain Band Gap

Compound	Hartree		Gap Energy (eV)
	HOMO	LUMO	
Betalain	-0.206058	-0.090199	3.152685477
Anthocyanin	-0.197554	-0.063061	3.659742686

From table 1, the data obtained from NwChem cannot be directly used to find the band gap value, because the unit of HOMO LUMO is still a Hartree. In determining the band gap using NwChem, the HOMO-LUMO data unit from the data must first be converted to eV. The results obtained are HOMO is -5.607126455 eV and LUMO is -2.454440978 eV. As in table 1, from the HOMO-LUMO data, the results of the band gap or energy range are 3.152685477 eV.

Researchers have also prepared results from the band gap of anthocyanins which are more often used as materials for DSSC. The results obtained are HOMO is -0.197554 and LUMO is -0.063061. then, the band gap obtained from anthocyanins is 3.659742686 eV.

Anthocyanin is one type of organic compound that can be used to make DSSC because both are organic dyes or natural pigment that has some similarities and similarities in several aspects. Therefore, anthocyanins are suitable to be used as a quality comparison of betalains. From the comparison results, it was found that the band gap of Betalain has almost the same number as anthocyanins, and the band gap of Betalain is lower than the band gap of anthocyanins, it is certain that Betalain has a higher level of effectiveness than Anthocyanins. Because the lower the energy gap, the easier it is for the compound to excite electrons and that means the higher the level of effectiveness when used as a material for DSSC.[9][10][11]

## CONCLUSIONS AND RECOMMENDATIONS

### Conclusions

The HOMO-LUMO band gap obtained from Betalain compounds is 3.152685477 eV. The HOMO-LUMO band gap obtained shows a fairly good result where this result is smaller than the band gap of the Anthocyanin compound, which means that Betalains are easier to excite electrons than Anthocyanins.

### Recommendations

It is necessary to conduct direct testing or experimental tests regarding the manufacture of Dye-Sensitized Solar Cell or DSSC using Betalain compounds from Binahong with a red trunk to test the computational theory that has been carried out. To realize the creation of a DSSC made from Binahong with a red trunk. That means Betalain has a higher level of effectiveness when used as a material for DSSC.

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