Tauc Plot Software: Calculating energy gap values of organic materials based on Ultraviolet-Visible absorbance spectrum

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Abstract. Studies on bio-organic materials for optoelectronic devices have increased recently, mainly due to the low cost of the materials. Electrical properties of the materials are important to review whether a material is suitable for optoelectronic applications. The energy gap is an important parameter to investigate the electrical properties of materials, and therefore, the band gap value has to be determined accurately. The energy gap of a semiconductor material can be calculated from its absorption spectrum using the Tauc plot method. In this article, we designed software based on the Tauc plot method (Taucplot4dotz) and ran a trial test using data from our previous studies on Sukun (Artocarpus Altilis) leaves extract and Gamal (Gliricidia Sepium) leaves extract. Results obtained were more accurate than our previous calculations since we used both horizontal dan vertical linear extrapolation lines compared to only one in our previous calculations. We also used re-fitted data of ZnO [26]. Our accurate and fast calculation using the software showed that energy gap values of Sukun leaves and Gamal leaves extract were 3.033 eV and 1.833 eV, respectively. For ZnO, the energy gap was found to be 3.6205 eV, slightly different from the original data (3.625 eV) [26]. From the results, it can be concluded that the software provides an easier and faster calculation of energy gap values of materials, from which one can further investigate the potential of the materials suitable for optoelectronic devices based on bio-organic materials. Keywords: tauc-plot method, organic materials, energy gap, Absorbance, UV-Vis Spectrum.

1. Introduction

Research on optoelectronic devices has increased recently. One of many important factors to investigate whether a material is suitable for optoelectronic applications is the electrical property of materials. In the field of material physics, one way to determine the electrical properties of a material is energy gap values. An energy gap is an energy region where the density of states of electrons is zero. As an energy region where electron cannot exist, the energy gap separates two allowed electronic energy states. These electronic energy states in materials instead of having discrete energies as in the case of a single atom, they form bands, namely the valence band and the conduction band. The valence band is the region where electrons occupy the outer states in atomic structure and is fully filled with electrons. Meanwhile, the conduction band is the region where electrons can move freely to generate electrical current and has higher energy than the valence band. Usually, the conduction band is empty,
but in the case of metals, it is partially filled. The energy region between these two bands forms a forbidden band known as the energy gap. The energy gap value is defined as the difference between the top of the valence band and the bottom of the conduction band and it can be used to determine whether a material is categorized as a metal, a semiconductor or an insulator. Metals do not have energy gap, meaning that the conduction band and the valence band overlap with each other so the electron can move freely from the valence band to the conduction band. On the other hand, semiconductors and insulators have energy gap, with values being less than 4 eV for the former and greater than 4 eV for the latter [1].

Calculations of material energy gaps have been carried out in many studies using various materials, including bulk materials, thin layers, bio-organic materials and nanomaterials [2-17]. There are various methods of calculating them, including the photoluminescence (PL) method [2-5], the Cody plot method [6,7,8], the Tauc plot method [9-20], and so on. The Tauc plot method is one of the most popular methods in calculating energy gap values. This is because the calculations are simple and accurate for amorphous materials [19, 20]. Calculation of energy gap using this method requires only UV-Vis Absorbance spectrum data.

In this study, software to calculate energy gap using the Tauc plot method is designed. The purpose of this design is to make the calculations faster and easier.

Tauc Plot Method was first developed by Tauc in 1968 [9]. This method gained popularity when research on thin layers began to develop rapidly [14-17]. At that time, scientists were competing to conduct experiments in searching for new materials.

Calculation of energy gap value using the Tauc Plot method is started by calculating the absorption coefficients ($\alpha$), namely the equation:

$$\alpha = \frac{A \ln(10)}{l}$$

(1)

where $A$ = Absorbance value from UV-Vis spectrometer and $l$ = sample width (cm).

In addition, the conversion of wavelength $\lambda$ (nm) into energy units $h\nu$ (eV) is also calculated using equation:

$$1 \text{ Joule} = 1 \ h\nu = \frac{hc}{\lambda} \times 6.241509 \times 10^{18} \text{ eV}$$

(2)

According to Tauc, the energy gap values can be obtained from the following equation:

$$(ah\nu)^{1/m} = B(h\nu - E_g)$$

(3)

where $h$ = Planck’s constant ($4.135 \times 10^{-15} \text{ eV.s}$), $\nu$ = frequency (s$^{-1}$), $B$ = a comparative constant, $E_g$ = energy gap (eV).

$m$ indicates the type of electronic transition, with values for different transitions being:

- $\frac{1}{2}$ = Direct
- $\frac{3}{2}$ = Direct forbidden
- 2 = Indirect
- 3 = Indirect forbidden

These $m$ values are used in the calculations and the one that yields the best fitting results is chosen as the ‘correct’ $m$ value [18], which can be used as a preliminary indication about the type of electronic transition in materials. However, to determine the type of transition accurately we need to use other experimental methods.

To evaluate equation (3), values of $(ah\nu)^{1/m}$ and $h\nu$ are calculated first. Then, the next step is to plot the results. The plot yields an irregular curve but there are some parts that are in the form of a straight or linear vertical line. In accordance with equation (3) where the value of $E_g$ must be directly proportional to the value $(ah\nu)^{1/m}$ then the equation applies to this linear part of the curve.
Next, in the linear part, extrapolation is carried out so that it cuts the $hv$ axis. The intersection of the extrapolation line with the $hv$ axis is the energy gap value ($E_g$) of the material of interest. In the modified Tauc plot method [19,20], a second extrapolation line is drawn from the horizontal direction, then the intersection between the two lines determines the $E_g$ value. This leads to more accurate $E_g$ values. Therefore, we apply this method in developing our software.

Extrapolation is a technique of estimating data from previously owned data. This extrapolation technique has been used in various fields of science [2-24]. The simplest extrapolation technique is a linear extrapolation technique where the value we want to find $f(x)$ is approached using the equation:

$$f(x) = f(x_n) + \frac{f(x_{n+1})-f(x_n)}{(x_{n+1}-x_n)}x$$

with $x_n$ = the value of $x$ to $n$, and $x_{n+1}$ = the value of $x$ to $n+1$.

In applying the modified Tauc plot method, two extrapolation lines are needed so that calculations with two equations are carried out. Then the intersection is searched, when the two lines intersect, we will get a combination of two equations, and the value of $x$ as $E_g$ can be determined:

$$f(x_1) + \frac{f(x_2)-f(x_1)}{(x_2-x_1)}x = f(x_3) + \frac{f(x_4)-f(x_3)}{(x_4-x_3)}x$$

$$f(x_1) + Mx = f(x_3) + Nx$$

$$E_g \approx x = \frac{f(x_2)-f(x_1)}{M-N}$$

where 1 and 2 are data points for extrapolating from the horizontal direction, whereas 3 and 4 are data points for extrapolation from the vertical direction.

2. Research Method
The development of the TaucPlot4dotz software [25] is divided into two stages, namely: Design and Trial.

2.1. Design
At this stage, a flow chart is created to apply the Tauc plot method. This flow chart can be seen in Figure 1. Calculations begin by entering input data in the form of wavelength ($\lambda$) and absorbance ($A$) data files which can be obtained from the results of UV-Vis spectrophotometer characterization of the sample. The data is then displayed and plotted on the screen.

The next step is to calculate the absorption coefficient values ($\alpha$) using equation 1 and also do the calculation of the wavelength conversion value from nanometer (nm) to the energy unit (eV) using equation 2. In addition, at this stage, the software calculates the $(\alpha hv)^{1/m}$ values in equation 3. The results of this calculation are displayed and then plotted vs energy ($E$).

The last step is to determine the linear area of the curve plotted and to choose four points (X1, X2, X3, and X4) which will be used to make two straight lines extrapolating from the horizontal and vertical directions (equation 4). The intersection of the two lines is calculated by equation 8 to obtain the energy gap value.

Graphic User Interface (GUI) of the software design can be seen in Figure 2.
2.2. Trial
At this stage software testing is carried out using sample data: ZnO (re-fitted data from [26]) and from previous studies on leaves extract [10,11], using the following steps:

- First enter the data by pressing the INPUT button and selecting the data format *.csv and obtain the first plot as shown in figure 3.A.
- Then calculate the absorption coefficients, the conversion of wavelength and \((ahv)^1/m\) by selecting the value of \(m\) and determining the sample length value first, then pressing the CALCULATE button. The results obtained are shown in figure 3.B, where the results of calculations and the second plot are shown.
- After the results are obtained, it is followed by determining the linear area of the curve from the second plot and calculating two extrapolation lines by specifying four points (specify the point from the table and press the X1H button to select, repeat for the next X2H, X1V and X2V). Choose these four points from the “linear area” of the curve. X1H and X2H are chosen from the horizontal part while X1V and X2V are chosen from the vertical part.
- After the selection, press the Energy Gap button to obtain the energy gap values. Examples of some results can be seen in Figure 3.C.

![Flowchart](image)

**Figure 1.** Flowchart of designing the TaucPlot4dotz software [24].
Figure 2. GUI of the TaucPlot4dotz software [24].
3. Results and Discussion

Calculation results for ZnO (re-fitted data from [26]) can be seen in Figure 4. ZnO absorbance spectrum was chosen because it has well-known energy gap value of 3.1 eV - 3.5 eV and the type of transition is direct transition [18]. Energy gap value of ZnO obtained from our calculation was 3.6206 eV, which is only slightly different from the original data result of 3.625 eV [26]. This result clearly showed that the software has good accuracies.

Other results of the data testing can be seen in Figure 5 and Table 1. The table shows six experimental data, namely three experimental data on the absorbance of Sukun (*Artocarpus Altilis*) leaves extract from Kassa, et al. [10] and three experimental data on the absorbance of Gamal (*Gliricidia Sepium*) leaves extract from Tedju, et al. [11]. From the data, the energy gap values were determined using the TaucPlot4dotz software.

![Figure 4](image1.png)

**Figure 4.** (A) ZnO Absorbance re-fitted data from [26], (B) ZnO Energy Gap Calculation Result using our software
Figure 5. (A) Sukun (*Artocarpus Altilis*) leaves extract, (B) Gamal (*Gliricidia Sepium*) leaves extract.

Table 1. Energy gap values comparison between calculation from Kassa et al. [10] and Tedju et al. [11] with Taucplot4dotz software.

| Types of extract | ppm in ethanol | Previous Calculation (eV) [10,11] | tauclplot4dotz (eV) |
|------------------|----------------|---------------------------------|-------------------|
| *Artocarpus Altilis* | 100            | 3.03                            | 3.066             |
|                  | 200            | 3.03                            | 3.042             |
|                  | 300            | 3.03                            | 3.030             |
| *Gliricida Sepium* | 200            | 1.832                           | 1.834             |
|                  | 300            | 1.832                           | 1.833             |
|                  | 400            | 1.831                           | 1.832             |

Energy gap values compared with the energy gap values from our previous calculations which only use one extrapolation line in [10,11] show that the values are quite similar. However, one of the main results here that differ from our previous results is that our results presented in this article are more accurate. According to Ehsan, et al [19] and Russel, et al. [20], the use of two extrapolation lines also provide more accuracy compared to one extrapolation line calculations.

To the best of our knowledge, there is no “Tauc plot specific” software, but Tauc plot method can be implemented with various plotter-calculation software. One of the advantages of the software we develop here over other software is that there is no need to apply the equation and plot the curve. Our software is faster and easier to use.
4. Conclusions
Results show that energy gap values can be calculated faster and easier using our software. The results also provide us with information of the possible types of electronic transitions. Finally, the results obtained here are also more accurate because of the use of the modified Tauc plot method [19,20].

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