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The Study of the Optical Characteristics of Materials for the Construction of Organic/Inorganic Solar Cells Using UV – VIS Spectroscopy

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Abstract: *This study focuses on the UV-vis spectroscopic analysis of the active materials used to construct organic/inorganic solar cells. The analysis was carried out on PCMB: P3HT blend using toluene as the solvent. It was also carried out on different concentrations of ZnO solution. The absorption spectra show that the PCMB-P3HT blend exhibited the highest absorption between 584.55 and 623.33 nm. The transmittance spectra show no transmission within the wavelength in which the absorption is at its peak. The highest peak is obtained at 617.81 nm in both the absorption and extinction coefficients. The blended material has a direct band gap value of the PCMB: P3HT blend is 1.94 eV. The Absorption spectra of 0.4ml-ZnO, 0.8ml-ZnO, and 1.2 ml-ZnO show that 0.8ml-ZnO exhibited different absorption and better absorbance than that of 0.4ml-ZnO and 1.2 ml-ZnO, which have similar absorption spectra with each other. But they all exhibited maximum absorption at almost the same wavelength, at about 343– 346nm. The optical band gap for 0.4ml ZnO was discovered to be 3.1 eV. While that of 0.8ml and 1.2ml ZnO are 3.0eV and 2.3eV respectively. These values indicated that as the concentration increases, there is an increase in the band gap.*

Keyword: *Organic photovoltaics, PCMB-P3HT, thin film, ZnO, UV-vis spectroscopic analysis.*

Introduction

Electrical energy generation using solar cells has received massive investment in its research, production, and deployment (Huyunh *et al*., 2002). Solar cells are semiconductor devices that can convert sunlight into electricity and are usually made of silicon. This material is used to produce solar cells because of its electronic properties, abundance, lack of toxicity, and high efficiencies and stabilities of the cells produced. In addition, solar cells made of silicon are the major product on the market because of their high power conversion efficiencies (PCEs), which reach up to 40% (Kali *et al*., 2012). However, high costs imposed by fabrication procedures involving elevated temperature (400° to 1400°C), high vacuum, and numerous lithographic steps have limited the widespread expansion in the use of silicon(inorganic) solar cells.

Organic photovoltaic solar cells (OPV) have become a promising candidate for achieving low-cost solar energy conversion devices. This is because they can be fabricated using simpler and cost-effective processing schemes, such as screen printing, inkjet printing, dip coating, and roll-to-roll processing (Pudasaini & Ayon, 2013).

Polymers used in OPV are characterized by being conjugated: the conjugation of a polymer refers to the presence of a backbone chain of alternating double and single bonds. The sp2 hybridized carbon centers

have a valence electron in the pz orbital (π), which is orthogonal to the other σ bonds. The overlapping of π/π bonds determines the creation of delocalized energy states within the structure. This promotes intermolecular transport and allows for the transport of charge.

Zinc Oxide (ZnO) is a member of II-VI semiconducting compounds and occurs naturally in mineral zincates. Zinc oxide nanoparticles play a great role in industrial areas because it has specific properties. These properties include excellent heat resistance, low electron conductivity, anti-bacteria, and anti-corrosion (Vishwakarma & Singh, 2020). Furthermore, as an n-type inorganic semiconductor, ZnO has been widely used in organic solar cells (OSCs) and hybrid solar cells (HSCs) due to its salient characteristics such as low cost, easy synthesis, non-toxicity, high stability, and good optoelectronic properties (Huang *et al*., 2011).

In this study, the UV – vis spectroscopy is used to analyze the materials used in the construction of the active region of an organic/inorganic hybrid solar cell.

Experimental Method

Highly Regioregular poly(3-hexylthiophene) P3HT (95.0%) and poly(3-hexylthiophene) PCMB (99.0%) and were purchased from Ossila. Both of them were a blended ratio of 0.6: 1. toluene was used to dissolve the two polymer materials at 25mg/ml. The dissolved blended material was deposited by spin coating on a glass slide in a normal atmosphere at room temperature.

For the synthesis of ZnO sol-gel technique is used. Zinc acetate dihydrate is used as a precursor and methanol as a reagent. Distilled water is used as a solvent. All chemical reagents in this experiment were obtained from commercial sources as guaranteed grade and were used as received without further treatment. 0.4ml of Zinc acetate dehydrate was dissolved in 50ml of methanol solution under continuous stirring at room temperature for 10 minutes. A few drops of acetic acid were added to the solution since the PH of zinc acetate was too high. Continuous stirring was applied until everything was dissolved. A solution of ZnO of different concentrations of 0.4ml-ZnO, 0.8ml-ZnO, and 1.2ml-ZnO was obtained using this method. The solutions were deposited on different substrates using spray pyrolysis.

UV–vis–NIR spectrophotometry (UV-750 Series) was used to characterize the optical characteristics of these materials.

Result and Discussion

The graphs below show the absorbance, transmittance, absorption coefficient, and optical energy bandgap of the PCMB: P3HT blend. Also displayed are the absorbance and optical energy bandgap of different concentrations of ZnO solutions. Figure 2 shows the absorption spectra of the PCMB: P3HT blend. The figure shows that the blended material exhibited the highest absorption between 584.55 and 623.33 nm. This shows that the material harvests light the highest at the previously mentioned wavelengths. However, there is little or no absorption in the red and NIR portion of the spectrum

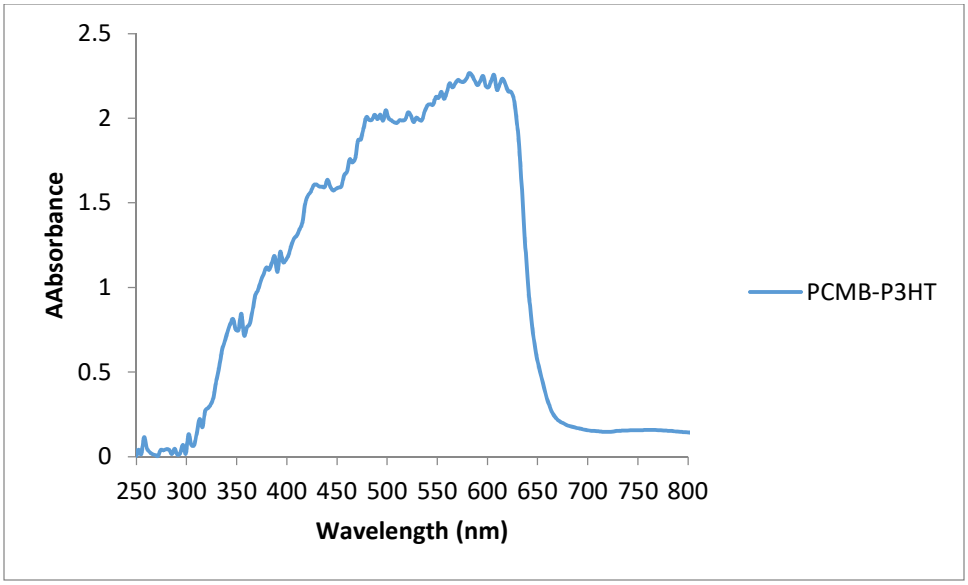

Figure 1 Absorbance of PCMB-P3HT blend

The transmission spectra of the PCMB: P3HT blend is displayed in figure 1. From the figure, it could be seen that the material exhibited very low transmittance, especially between 400 – 635 nm. This is the opposite of absorption spectra. Hence, dissolving the blend in toluene reduces visible light transmission between these wavelengths.

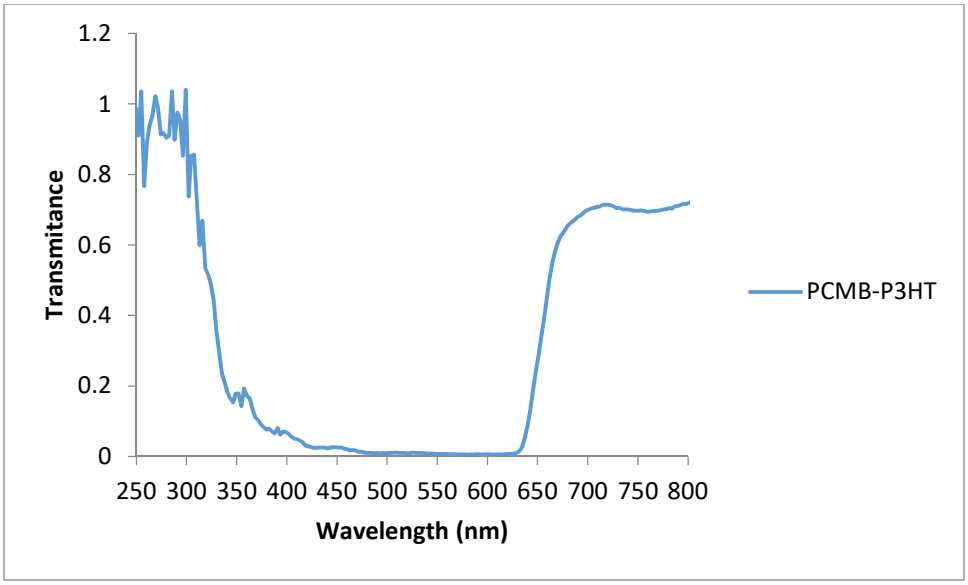

Figure 2 Transmittance spectra of PCMB-P3HT blend

Looking at figure 3, the graph of the absorption coefficient of the blended dissolved blended material corresponds with the absorption spectra. The absorption coefficient was obtained using the relation (King & Milosevic, 2012),

$\alpha = 2.304 \text{ x } A/t$ 1

Where A is the absorbance and t is the thickness of the film.

There is an increase in the absorption coefficient between 400 – 635 nm. However, between 250 - 300 nm, the material exhibits little to no absorption. The same is also observed in figure 5, which is the extinction coefficient of the blended materials. The highest peak is obtained at 617.81 nm in both the absorption and extinction coefficients.

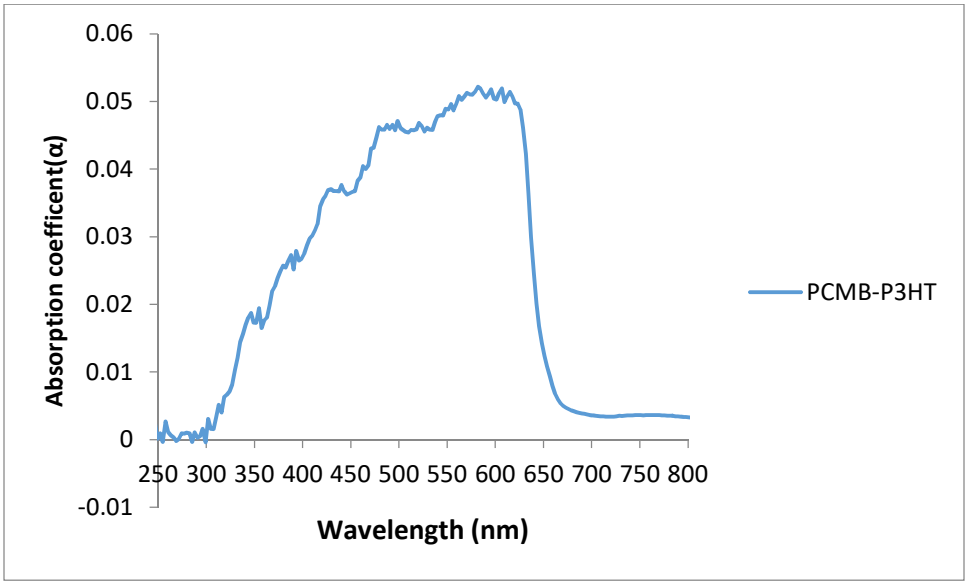

Figure 3 absorption coefficient versus the wavelength of PCMB-P3HT blend

The absorption spectra of the different concentrations of ZnO are shown in figure 4. The graph shows that the samples exhibited maximum absorption at almost the same wavelength, at about 343– 346nm. However, the Absorption spectra of 0.4ml-ZnO, 0.8ml-ZnO, and 1.2 ml-ZnO show that 0.8ml-ZnO exhibited different absorption and better absorbance than that of 0.4ml-ZnO and 1.2 ml-ZnO, which have similar absorption spectra with each other.

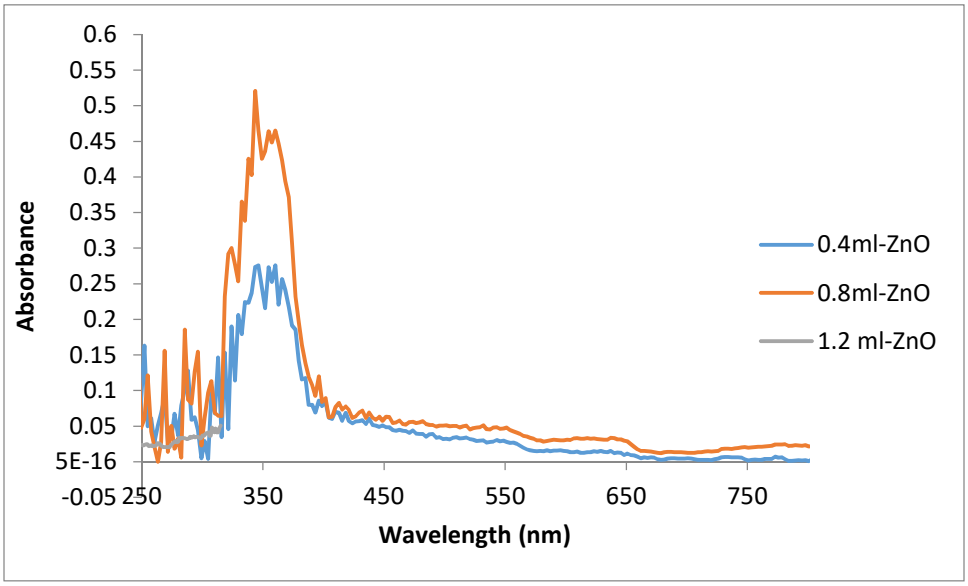

Figure 4 Absorption spectra of 0.4ml-ZnO, 0.8ml-ZnO and 1.2 ml-ZnO semicoductor

The optical energy band gap is obtained from the graph in figure 6. The graph is a plot of $(\alpha h\nu)^2$ as a function of photo energy. The optical energy bandgap E_g of indirect band gap materials is evaluated using the relation,

$$\alpha h\nu = \left[A\left(h\nu - E_g\right)\right]^2 \quad 2$$

Where A is a constant, $h\nu$ is the photon energy, and α is the absorption coefficient.

The difference between the optical and electrical energy band gap is that the electrical band gap is the minimal energy required to create an electron-hole pair in a semiconductor. In contrast, the optical band gap is the exciton energy determining the onset of vertical interband transitions.

An exciton is a bound state of an electron and hole held together by the electrostatic Coulomb force; an exciton forms when a semiconductor absorbs a photon. So therefore, the optical band gap is the threshold for photons to be absorbed.

By extrapolating the straight portions of the graphs on the hν axis, the bandgaps were obtained from the intercepts since $E_g = h\nu$, when $\alpha h\nu = 0$. Figure 8 shows that the direct band gap value of the PCMB: P3HT blend is 1.94 eV.

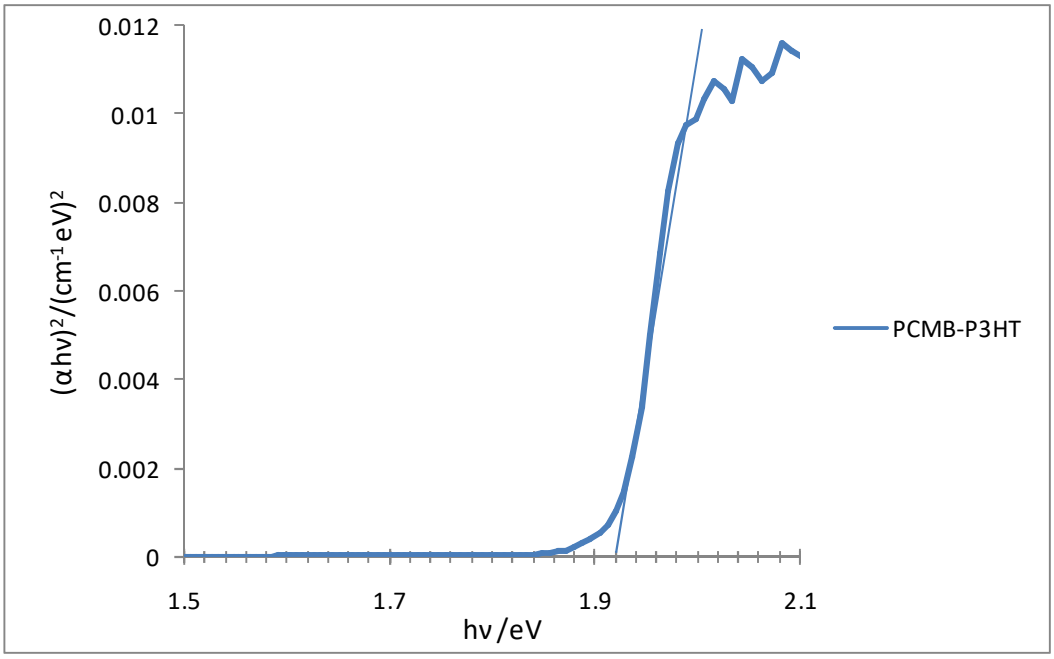

Figure 5 Bandgap spectra for PCMB: P3HT blend

Figures 9, 10, and 11 represent the optical band gap values of 0.4ml, 0.8ml, and 1.2ml ZnO, respectively. The optical band gap is different from the electrical or electronic band gap. The electronics on electrical band gap is the energy the electrons require to move from the semiconductor's conduction band to the valence band. In contrast, the optical band gap is the energy at which a material starts absorbing photons. For example, ZnO is a direct semiconductor, and its absorption coefficient (α) and incident photon energy(hυ) is related with the following equation (Tauc *et al*., 1966):

$$(\alpha h\nu) = A(h\nu - E_g)^{\frac{1}{2}} \quad 3$$

The optical band gap for 0.4ml ZnO is discovered from the graph to be 3.1 eV. While that of 0.8ml and 1.2ml ZnO are 3.0eV and 2.3eV respectively. These values indicate that as the concentration increases, there is an increase in the band gap.

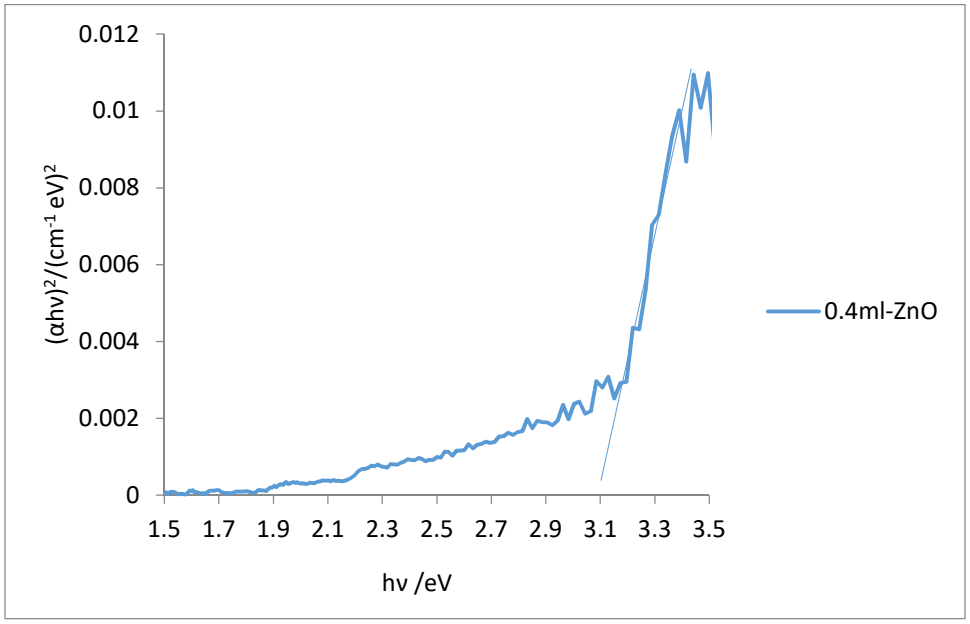

Figure 6 Bandgap spaectra for 0.4ml-ZnO

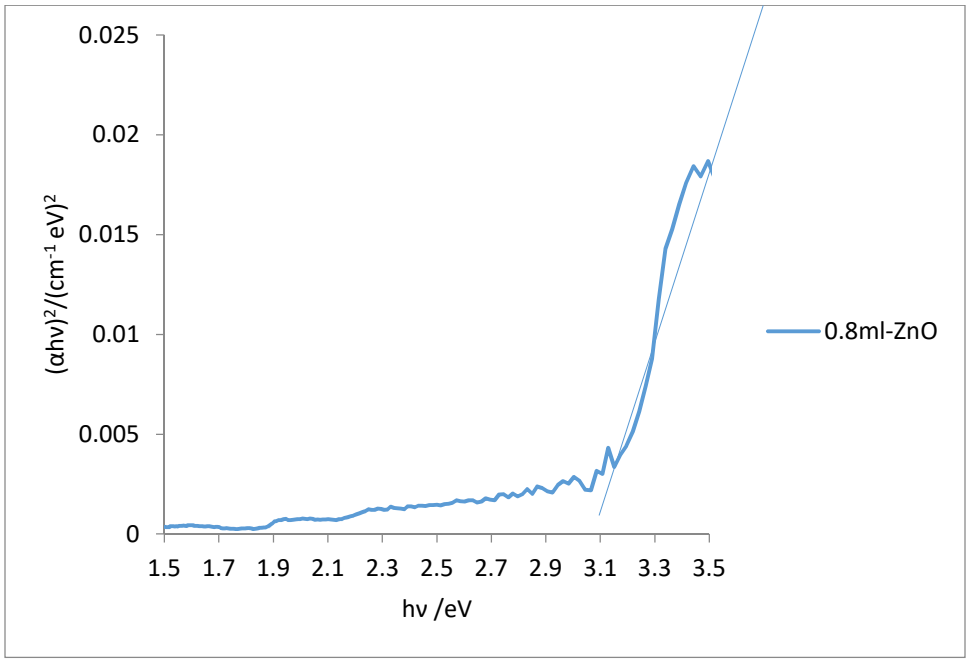

Figure 7 Bandgap spaectra for 0.8ml-ZnO

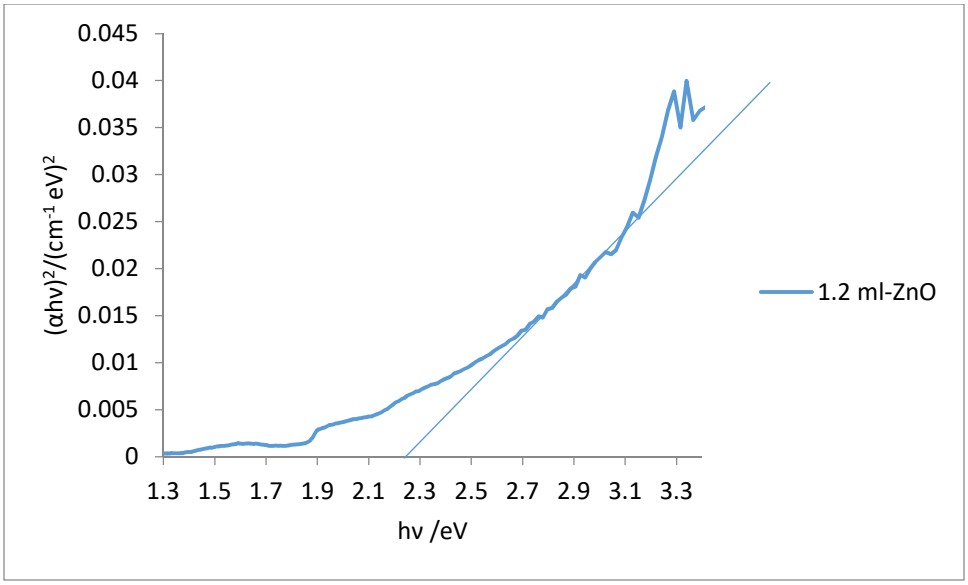

Figure 8 Bandgap spaectra for 1.2ml-ZnO

Conclusion

This paper determined the optical characteristics of the active materials required to construct organic/inorganic polymer solar cells using a UV-vis spectroscope. The absorption spectra show that the PCMB-P3HT blend exhibited the highest absorption between 584.55 and 623.33 nm. The transmittance spectra show no transmission within the wavelength in which the absorption is at its peak. The highest peak is obtained at 617.81 nm in both the absorption and extinction coefficients. The blended material has a direct band gap value of the PCMB: P3HT blend is 1.94 eV. The Absorption spectra of 0.4ml-ZnO, 0.8ml-ZnO, and 1.2 ml-ZnO show that 0.8ml-ZnO exhibited different absorption and better absorbance than that of 0.4ml-ZnO and 1.2 ml-ZnO, which have similar absorption spectra with each other. But they all exhibited maximum absorption at almost the same wavelength, at about 343– 346nm. The optical band gap for 0.4ml ZnO was discovered to be 3.1 eV. While that of 0.8ml and 1.2ml ZnO are 3.0eV and 2.3eV respectively. These values indicated that as the concentration increases, there is an increase in the band gap.

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