Faculty of Resource Science and Technology

POTENTIAL APPLICATION OF BIS-CHALCONE IN PLASTIC SUBSTRATE SOLAR CELL DEVICE

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Potential Application of Bis-chalcone in Plastic Substrate Solar Cell Device

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Declaration

I declare that the work in this thesis was carried out in accordance with the regulations of Universiti Malaysia Sarawak. It is original and is the result of my work, unless otherwise indicated or acknowledged as referenced work. This thesis has not been submitted at this or any other university or academic institution for any other degree or qualification.

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List of Abbreviation

$AlCl_3$	Aluminium chloride
$Ba(OH)_2$	Barium hydroxide
CdS	Cadmium sulfide
CdTe	Cadmium telluride
CH_3OH	Methanol
$CHCl_3$	Trichloromethane
CIGS	Copper indium gallium diselenide
CIS	Copper indium selenide
Cl^-	Chloride ion
Cs_2CO_3	Cesium carbonate
DCM	Dichloromethane
DMF	Dimethylformamide
DMSO	Dimethylsufoxide
DSSC	Dye-sensitized solar cell
E_g	Energy band gap

FTIR	Fourier transform infrared
H_2O	Water molecule
HCl	Hydrochloric acid
I^-	Iodide ion
I_3	Triiodide ion
KBr	Potassium bromide
KI_3	Potassium triiodide
KOH	Potassium hydroxide
MeCN	Acetonitrile
$Na_2S_2O_3$	Sodium thiosulfate
NaOH	Sodium hydroxide
Ni	Nickel
$Ni(II)Cl_2 \cdot 6H_2O$	Hexaaquanickel(II) chloride
NLO	non-linear optics
NMR	Nuclear magnetic resonance
OH^-	Hydroxide ion
$Pd(PPh_3)_4$	Tetrakis(triphenylphosphine)palladium(0)

PET	Photoinduced electron transfer
Pt	Platinum
Ru	Ruthenium
SHG	second harmonic generation
$SOCl_2$	Thionyl chloride
STC	Standard test condition
TCO	Transparent conducting oxide
THF	Tetrahydrofuran
$TiCl_4$	Titanium chloride
TiO_2	Titanium dioxide
TLC	Thin layer chromatography
UV-Vis	Ultraviolet-visible

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Abstract

Due to depletion of petroleum, global is seeking for renewable energy to replace the conventional energy. In this study, plastic solar cell was developed by using bis-chalcone (1,4-bis[2-(2-hydroxybenzoyl)vinyl]benzene) as a dye. Bis-chalcone was successfully synthesized by base-catalytic Claisen-Schmidt condensation between 2-hydroxyacetophenone and terephthalaldehyde. The synthesized bis-chalcone was characterized using FTIR and NMR spectroscopy. After that, bis-chalcones were coated on spin coated and hand coated TiO_2 which show 3.601 x 10^{-3} % and 2.439 x 10^{-3} % of efficiency respectively. Besides, CuS was successfully coated on plastic substrate by using chemical bath deposition and the resistance per cm square of plastics substrate showed 74.6, 31.1 and 12.5 Ω cm^{-2} when 0.01, 0.05 and 0.10 M of precursors were used respectively. Apart from that, plastics substrate solar cells were fabricated based on 0.01, 0.05 and 0.10 M of concentration which showed 1.503 x 10^{-3}, 6.269 x 10^{-4} and 1.575 x 10^{-3} % of efficiency respectively. It is found that the 0.10 M against the theoretical hypothesis, which caused by a few factors included the improvement of plastics substrate conductivity, the properties of CuS and thermal barrier of bis-chalcone compound.

Keyword: Claisen-Schmidt condensation, bis-chalcone, plastic solar cell

Abstrak

Disebabkan petroluem yang semakin berkurangan, seluruh dunia sedang mengkaji tenaga yang dapat diperbaharui untuk mengganti tenaga asli. Dalam kajian ini, sel suria plastik telah diperkembangkan dengan menggunakan bis-chalcone (1,4-bis[2-(2-hydroxybenzoyl)vinyl]benzene) sebagai pencelup. Bis-chalcone telah berjaya dihasilkan secara sintesis dengan menggunakan dasar pemangkin Claisen-Schmidt pemeluwapan antara 2-hydroxyacetophenone dan terephthalaldehyde. Bis-chalcone yang disintesis mengambarkan sifatnya dengan menggunakan FTIR dan NMR spektroskopi. Selepas itu, bis-chalcones telah diselaputi atas penyelaput pusing dan penyelaput secara tangan TiO_2*, ia menunjukkan efisien 3.601 x* 10^{-3} *% dan 2.439 x* 10^{-3} *% masing-masing. Selain itu, CuS telah berjaya diselaputi atas plastik substrat dengan menggunakan mandian pemendapan kimia dan rintangan untuk plastik substrat bagi setiap empat persegi sentimeter adalah 74.6, 31.1 and 12.5 Ω* cm^{-2} *apabila 0.01, 0.05 dan 0.10 M perintis telah digunakan masing-masing. Di samping itu, sel-sel suria yang berplastik substrat telah difabrik dengan perintis yang berpekatan 0.01, 0.05 dan 0.10 M dan menunjukkan 1.503 x* 10^{-3}*, 6.269 x* 10^{-4} *and 1.575 x* 10^{-3} *% effisiensi masing-masing. Kajian ini mendapati bahawa 0.10 M bertentangan dengan hipotesis dari segi teori, ini boleh disebabkan oleh beberapa faktor, contohnya, pembaikan perihal pengaliran elektrik tentang plastik substrat, sifat CuS dan terma penyekat tentang bis-chalcone campuran.*

Kata Kunci: Claisen-Schmidt pemeluwapan, bis-chalcone, sel solar plastik

1.0 Introduction

Human are depending on energy to sustain their life. Fuel from fossil fuels was used in transportation and generates electricity for our daily uses. However, fossil fuel is not a renewable energy and might be used up in future. According to Muda and Tey (2012), Klass model forecasted that all the fossil fuels will be used up in 2077. Due to the depletion of petroleum, rising of fuels price and concerns with global warming when keep using fossil fuels as the primary energy source, many countries are looking for other renewable energy such as solar energy and hydro energy to replace fossil fuels. Renewable energy is generally defined as energy from non-depletable resources or resources that can be naturally replenish. Solar energy is one of the renewable energy that derived from sunlight. According to Smalley (2009), there is $3x10^{24}$ J per year of energy supplied from the sun to the earth, which is 10000 times more than what human uses. Therefore, it has the resource potential to become global energy demand as it is widely distributed on Earth's surface and causes no pollution to environment. Thus, development of solar cell that used to harvest solar energy has attracted a great attention in recent year.

The history of solar cell started in 1839 year when Becquerel observed that silver chloride coated platinum electrode in an aqueous nitric acid electrolyte generated direct current when the electrode is exposure under sunlight. Few decades later, Adams and Day (1876) observed that the solid state of selenium is able to generate electric current when exposure by light. However, due to the very low efficiency of conversion from solar energy to electrical energy, the electricity generated is not enough to operate electrical equipment. After the law of photovoltaic effect was discovered in 1905 by Einstein, Chapin and his coworkers developed the first silicon photovoltaic cell at the Bell Telephone Laboratory, USA. The efficiency of energy conversion for this photovoltaic cell achieved 6% (Bubenzer & Luther, 2003; Chapin *et al*., 1954; Fahrenbruch & Bube, 1983). Due to this high percentage of efficiency in energy conversion, the solar cells are able to generate enough electricity to operate electrical equipment. Besides, this new invention also acts as power sources in the field of astronautics, especially for satellites. However, these solar cells are only limited for the space applications, due to its high production costs. The commercial solar age is officially begun in 1954. Today, solar cells that widely used in the market, especially in microelectronic market are dominated by silicon type solar cell (Goetzberger *et al*., 2002).

1.1 Harvesting energy from light

Light is a form of energy which travels in the form of wavelength (**Figure 1.1**). Different wavelengths have different energy contents. The shorter the wavelength of light, the higher the energy content is. When light travels, the energy (light energy) is carried by elementary particles called photons. After the law of photovoltaic effect was discovery, scientists develop devices that can harvest the energy from light, which is commonly known as solar cell.

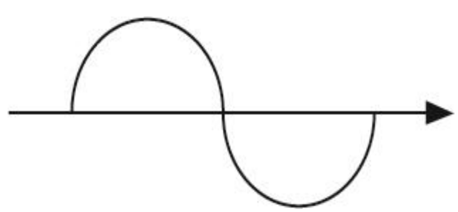


Figure 1.1: Wavelength of light

The efficiency of energy conversion is defined as the ability to convert solar energy into usable electricity. It is usually measured under standard test condition (STC). The STC refers to 1000 Wm^{-2} of sunlight irradiation and cell temperature of 25°C under air mass 1.5 (Arndt & Puto, 2011). It can be expressed in term of percentage as described by **Equation 1.1** (Emery & Osterwald, 1986):

$$\eta = \frac{P_{max}}{A \ x \ E_{STND}} \ x \ 100 \ \% \qquad \text{..........................} \textbf{Equation 1.1}$$

Where, η = conversion efficiency of solar cells under standard test condition

P_{max} = maximum power produced by solar cell in unit of watt, W

A = total surface area of solar cells (including frame and borders) in the unit of square meter, m^2

E_{STND} = standard spectral irradiance, 1000 Wm^{-2}

The maximum power cannot determine directly from the solar sell. It is determined by the product of fill factor (*FF*), short circuit current (*Isc*) and open circuit voltage (*Voc*) of solar cell (**Equation 1.2**).

$$P_{max} = FF \ x \ Isc \ x \ Voc \qquad \text{..........................} \textbf{Equation 1.2}$$

The power of solar cell is obtained when the value for both of the short circuit current and open circuit voltage is zero. Therefore, a term called “fill factor” is used as the parameter in conjunction with short circuit current and open circuit voltage in order to determine the maximum power of solar cell. Fill factor is defined as the ratio of maximum power from the sun to the product of short circuit current and open circuit voltage (Castellano, 2010).

According to Green (1981), fill factor can be calculated by using **Equation 1.3**.

$$FF = \frac{Voc - \text{In}(Voc + 0.72)}{Voc + 1} \qquad \text{……………………….……...…..} \textbf{Equation 1.3}$$

By combining the **Equation 1.1**, **Equation 1.2** and **Equation 1.3**, **Equation 1.4** is formed. In this study, **Equation 1.4** is used to calculate the conversion efficiency.

$$H = \frac{[Voc - \text{In}(Voc + 0.72)]\ x\ Isc\ x\ Voc}{A\ x\ E_{\text{STND}}\ x\ [Voc + 1]}\ x\ 100\ \% \qquad \text{………..} \textbf{Equation 1.4}$$

1.2 Chalcone compounds

Chalcone is a natural compound which can be found in apple seeds (Marcus *et al*., 2001). It is also known as benzalacetophenone or benzylideneacetophenone with the IUPAC name of 1,3-diphenyl-2-propen-1-one. The structure of chalcone (**Figure 1.2**) consists of two aromatic rings that linked by α,-β keto-enol containing group.

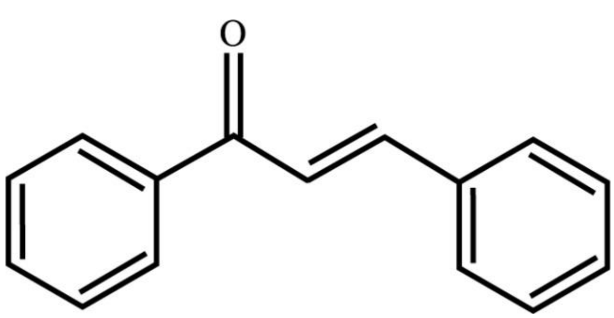
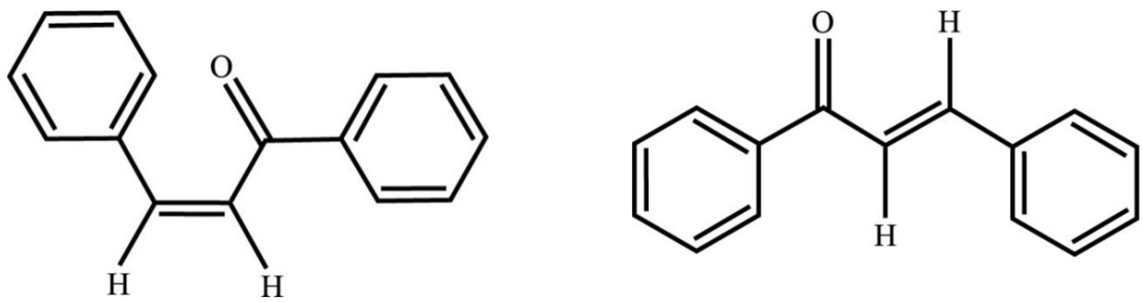


Figure 1.2: Structure of chalcone

Chalcone can exist either in *cis*- or *trans*- conformation (**Figure 1.3**) as the conjugated C-C double bond is present in the structure. *Trans*-conformation of chalcone is more thermodynamically favoured in normal condition due to the conjugated π-electron-system that leads to a stable and planar structure (Muller, 2012).



(a) (b)

Figure 1.3: (a) *cis*-chalcone; (b) *trans*-chalcone

Chalcone and its derivatives are widely used in materials science fields such as non-linear optics (NLO), optical computing, optical communication, optical limiting, photoinitiated polymerization, electrochemical sensing and Langmuir films (Asiri & Khan, 2011; Asiri *et al*. 2013). Chalcones are used as NLO due to its good optical power limiting properties and third-order nonlinearity (Kamath *et al*., 2014). They offer large nonlinear coefficients due to the fact that they consist of a conjugated double bond in between two planar benzene rings. The delocalization of π-electrons within these double bond and benzene rings are the one that responsible for the third order nonlinear optical responses (Poornesh *et al*., 2009). Furthermore, the responses can be increased by enhancing the ability of electron donating groups.

Besides that, some of the chalcone compounds have second harmonic generation (SHG) properties (Patil *et al*., 2007). SHG is a nonlinear optical process which a photon is produced from two photons with same frequency and energy in a nonlinear material. The produced photon has twice the frequency and amount of energy compared to the initial photons. Moreover, the wavelengths of the produced photons are only half of their initial photons (**Figure 1.4**). This nonlinear optical process allows the laser industry to make a stronger laser light. The incident laser with lower energy, less intensity and longer wavelength is able to convert into a stronger laser ray with higher energy, more intensity and shorter wavelength.

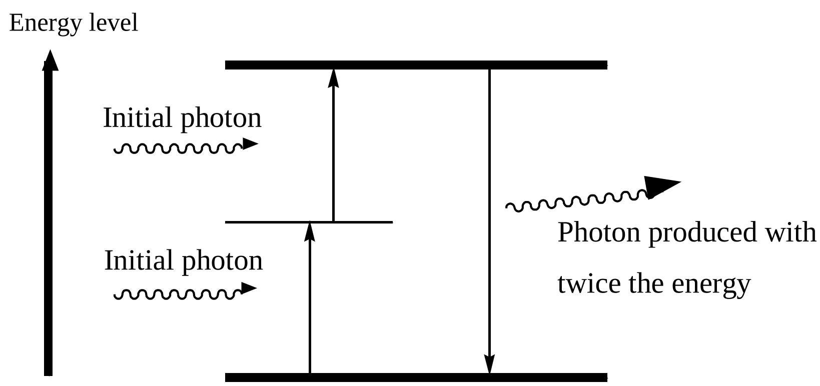


Figure 1.4: Second harmonic generation principle

Chalcone and its derivatives also play an important role in biological field especially for pharmalogical activities such as anti-bacterial, anti-malarial, anti-cancer, anti-microbial, anti-oxidant and anti-inflammatory (Prasad *et al*., 2008; Rahman, 2011). According to Syam *et al*. (2012), some chalcone derivative compounds such as 3-(4-Methoxyphenyl)-1-phenylpropenone having anti-cancer activity due to their capacity to elicit apoptosis. 3-(4-methoxyphenyl)-1-(4-pyrrol-1-yl-phenyl) prop-2-en-1-one (**Figure 1.5**), one of the chalcone derivative compound was used in anti-malarial which shows about 50% of inhibition concentration of the parasites stain (Awasthi *et al*., 2009). Besides, bis-pyrazoline that derived from bis-chalcone is used in anti-bacterial activities. This compound is able to inhibit both Gram-positive and Gram-negative bacteria (Asiri & Khan, 2011).

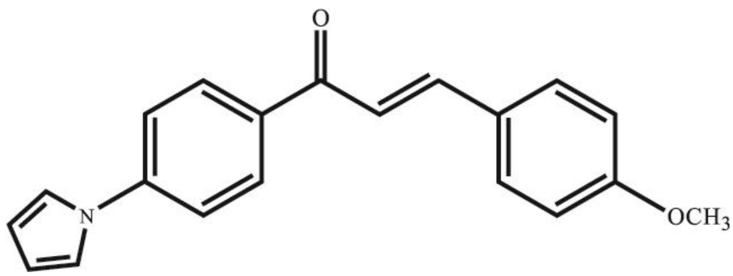


Figure 1.5: 3-(4-methoxyphenyl)-1-(4-pyrrol-1-yl-phenyl) prop-2-en-1-one

Due to the widely used of chalcone and its derivative compound, it is commonly synthesized artificially rather than extract from plants. Claisen-Schmidt condensation reaction is one of the common methods used in the synthesis of chalcone. Besides, microwave irradiation, ultrasound irradiation, Suzuki reaction and solvent-free grinding technique are also used in the synthesis of chalcone (Zangade *et al.*, 2011).

1.3 Photovoltaic solar cells

Photovoltaic solar cell is part of solar power system that converts sunlight into electricity. According to Saga (2010), there is about 90% of solar cells used in the market are made from silicon, it is known as conventional solar cell and built up by two layers of semiconductor, which are positive semiconductor (p-type) and negative semiconductor (n-type). Both p-type and n-type semiconductor are produced by the doping of silicon and joining together to form a p-n junction (**Figure 1.6**). When there is no current flow, a depletion layer is form in between the p-n junction. When the equilibrium has been achieved, there are negative ions (free electrons) in the p-type material and positive ions (empty holes) in the n-type material.

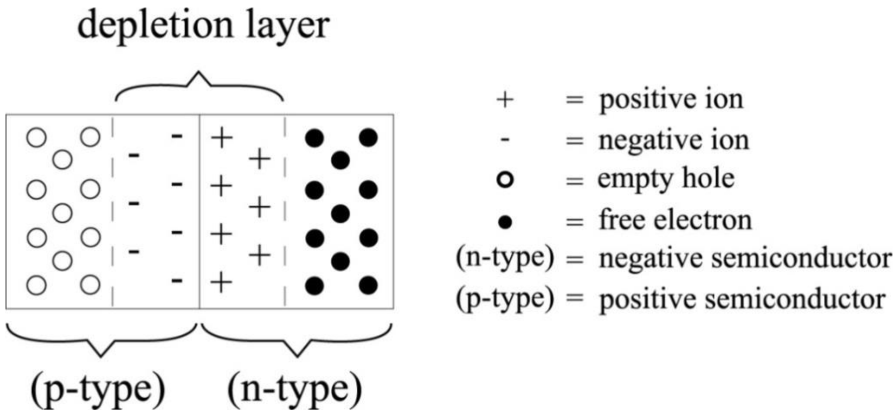


Figure 1.6: p-n junction

When the semiconductor is exposed under light, the valence electrons that weakly bonded to the nucleus absorbed sufficient energy and moved away from their particular position toward a conduction band. This results in the formation of positive holes (**Figure 1.7**).

a)