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CHARACTERIZATION OF QUINOLINE AND QUINOLINE CONJUGATED METAL AS THE BASE MATERIAL OFPHOTODETECTOR

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Abstract

Research has been conducted with the aim to characterize quinoline and quinolineconjugated metal as the base material of photo-detector. The characterization was conducted on the bandgap and infrared, visible, and ultraviolet spectra. This is done through computational chemistry method with NWCHEM 6.3 software. The computation is done by using density functional theory with basis set 6.31G*. The result showed that there was a diminution in the bandgap of quinolone conjugated metal of Mg(E_g ~ 0.16), Ca (E_g ~ 1.25), Cr(E_g ~ 3.51), Fe (E_g ~ 0.37), Ni (E_g ~ 1.18) and Zn (E_g ~ 3.58) than the bandgap of quinoline (E_g ~ 4.58 eV). Photosensitivity of the quinolin conjugated metalseem to shift towards the maximum wavelength in the visible and infrared, ie Mg-quinoline (λ_{max}= 470.57 nm); Ca-quinoline (λ_{max}= 719.98 nm); Cr-quinoline (λ_{max}= 855.76 nm); Fe-quinoline (λ_{max}= 1764.39 nm); Ni-quinoline (λ_{max}= 1325.20 nm); dan Zn-quinoline (λ_{max}= 485.04 nm), compare quinolone photosensitivity that occurs in the ultraviolet region (λ_{max}= 214.39 nm).

Keyword: Quinoline, conjugated metal, photo-detector, characterization.

1. Introduction

Optical sensors is very important in industrial automation systems. Such sensors work based on light sensitivity (Candra, 2006).Optical sensors are generally made by using semiconductor properties of inorganic materials, such as silicon and germanium (Setiawan et al, 2007).The characters of inorganic sensors are rigid, inflexible, limited amount of the deposit, and not easily recycled so it is not environmentally friendly.

Materials of organic compounds have not widely used as a semiconductors which become the raw materials of optical sensors. Though many organic compounds contain group that are active light. Organic semiconductors have such a chromophore groups is very prospective used as raw material of optical sensors.

Many adventages of the use of organic semiconductors as raw material for optical sensors. The structure of organic semiconductor is more flexible because the molecules have Van derWalls bonds. The flexibility of this structure is very important in industrial automation, especially in replacing mechanical works. In addition, the presence of organic material very abundant than inorganic materials which amount are very limited. Organic material is more easily recycled so it does not produce environmental pollution.

Organic materials which are potentially used as organic semiconductors for raw materials of optical sensors, is a material of organic compounds which have conjugated double bonds such as quinoline and others. Conjugated double bonds in organic compounds that allow the absorption of electromagnetic waves to move electrons from ground state to the excited state.

The existence of the chromophore groups and conjugated double bonds lead to organic semiconductors is potentially used as an infrared sensors and a light sensors in the range of UV-

Vis spectra (Pedersen et al, 2004). The sensitivity to light is closely related to the band gap of organic semiconductors that have conjugated double bonds (Brütting, 2005). Organic semiconductors with small band gap have large absorption to the electromagnetic wave.

Organic materials in general have a large band gap. The material is not quite ideal as semiconductors. To improve the properties, organic compounds in the sensor material need to be conjugated with metals. Good use is a metal that has empty d orbitals that electronic transitions can occur more easily (Pamungkas dan Sanjaya, 2013).

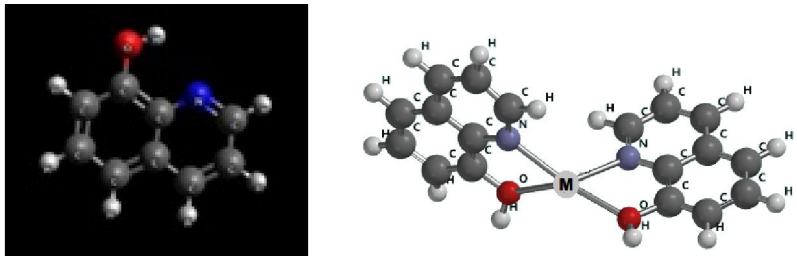
The research is focused on studying the semiconductor character of the derivative compound of quinoline and quinoline conjugated metal as the raw material of the optical sensors. The derivative qompound of quinoline which used as organic semiconductor are 8-hydroxyquinoline and 8-hydroxyquinoline conjugated metal. Under the terms of the ease electrons movement, the metal used in this study are the metals of Group IIA and the metal of periode 3. This selection is useful to determine the contribution of the metals periodically to improve the semiconductor quality of conjugated organic compounds. Studies conducted theoretically through computation chemistry performance.

2. Method

Modeling quinoline and metal quinoline were performed using the Avogadro 1.1.0. The development of the model is done by considering the possibility of coordination covalent bonds involving d orbitals of group IIA metals and metals of period 3. The model is converted into the input file of computation chemistry with program of gabedit 2.4.7. Computing process is then run using NWCHEM 6.3. Computational chemistry is carried out based on density functional theory with the basis set 6-31G*/B3LYP/Restricted Kohn-Sam (RKS). Band gap is determined using the difference between LUMO and HOMO energies. The absorption of light the virtualized with Spartan program.

3. Result and Discussion

Modeling quinolineandmetal-quinolinewhich is done by using Avogadro, shown in Figure 3.1. The notation M in the center is metal marking, which is conjugated to the quinoline structures.



a. Quinoline **b. Metal-Quinoline**

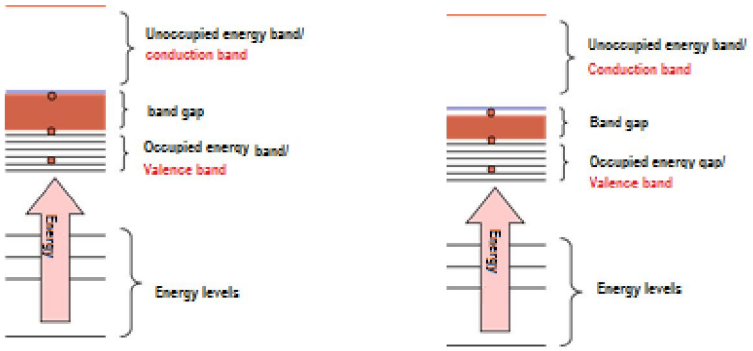
Figure3.1 The basic structure of Quinoline and Metal-Quinoline.

The band gap computation result of quinoline andmetal-quinoline in Figure 3.1showed a decrease in band gap of quinoline into quinoline conjugated metals.

Table 3.1The band gap result of Quinoline andMetal-Quinoline

Compound	HOMO-LUMO Energy (eV)		Band gap (eV)
	HOMO Energy	LUMO Energy	
Quinoline	-1.46458	-6.04240	4.57782
Mg-Quinoline	-2.48919	-2.64952	0.16033
Ca-Quinoline	-12.43888	-13.68823	1.24936
Cr-Quinoline	-12.64305	-16.15032	3.50727
Fe-Quinoline	-13.39013	-13.76018	0.37006
Ni-Quinoline	-14.13851	-15.32044	1.18193
Zn-Quinoline	-11.96226	-15.53794	3.57568

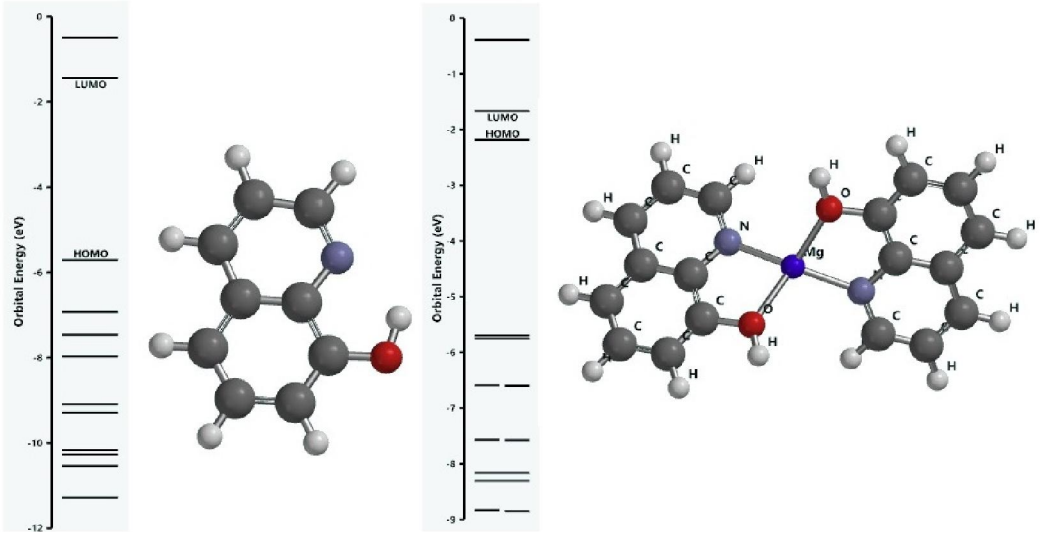
The decrease in the band gap is related to the narrowing gap between the valenceband and the conduction band. This is shown by band gap models in Figure 2. Valence band is indicated by the charging of the pile of orbitals in the HOMO groups and the conduction band is shown with a pile of the orbitals in the LUMO groups (Sanjaya et al, 2013).



(a) (b)

Figure 3.2.Band gap model of(a) quinolineand(b) metal-quinoline

This is made clear by the energy band structure of quinoline computational result and an example of metal-quinoline computational result which is represented by Mg-quinoline as shown in Figure 3.3.



(a) Quinoline (b) Mg-Quinoline

Figure 3.3. Band energy of Quinoline(a) andthe example of Metal-Quinoline (b)

The study could not show a decrease in band gap periodically for quinoline conjugated metals of group IIA and metals of period 3. There are few data on quinoline conjugated metal of group IIA. So it seemed only increase in band gap of Mg-quinoline into Ca-quinoline. While data from computational result of quinoline conjugated metals of period 3 shows the fluctuating band gap width.

Of the seven models of organic semiconductors which is computed, there are two compounds that are close to band gap of the silicon standard semiconductor (Gadisa, 2006),namely Ni-quinoline (E_g ~ 1.18 eV) and Ca-quinoline (E_g ~1.25 eV). There are two compounds that have band gap is smaller than the band gap of silicon, ie Mg-Quinoline (E_g ~0.16 eV)and Fe-Quinoline (E_g ~0.37 eV), so it is expected to work indoor.

Virtualization indicate that the computational results are accurate. These results are very similar to the standard. In Figure 3.4 is shown a comparison between computational result of infrared absorption of quinoline and the experimental result standard of infrared absorption of quinoline.

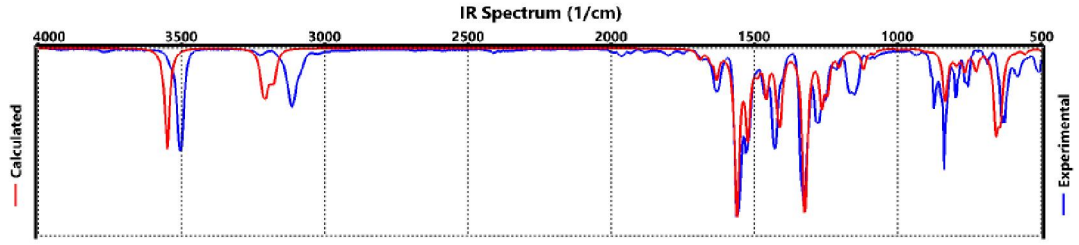
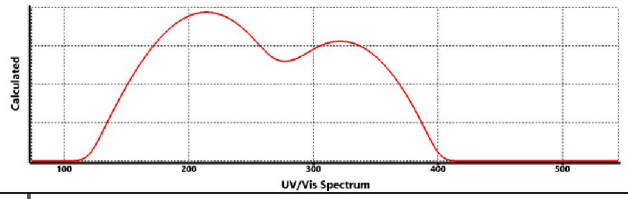
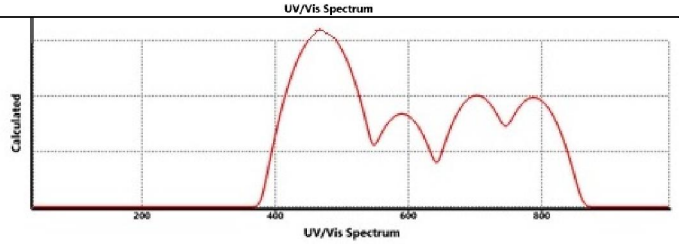
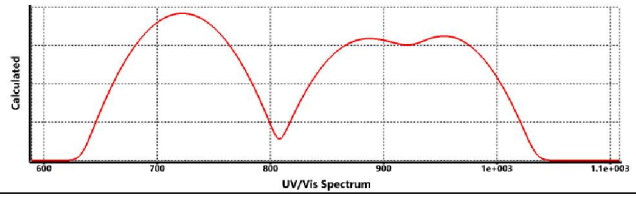
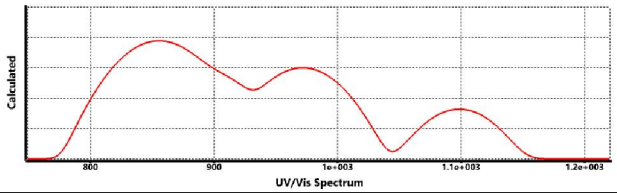
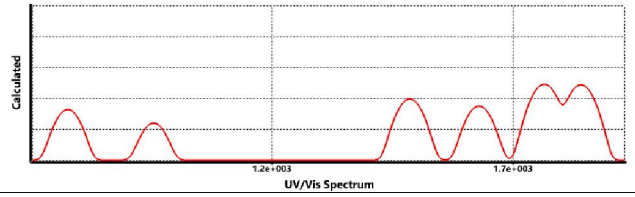
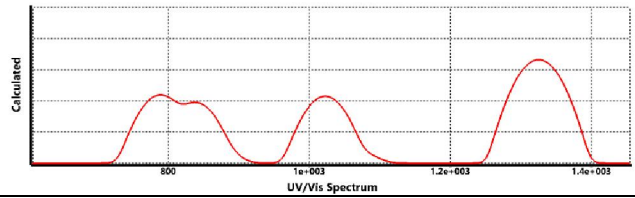
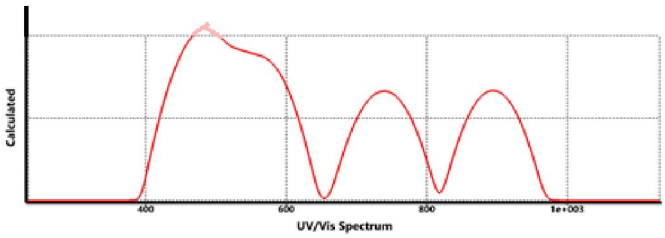


Figure 3.4. Infrared spectrum of quinolinefrom computation and standardof experimental result

The computational results of ultraviolet and visual absorptions of quinoline dan quinoline conjugated metal shown by table 3.2.

Table 3.2.Spectrum Uv-Viz of Quinoline andMetal-Quinoline

Quinoline	:	
Mg-Quinoline	:	
Ca-Quinoline	:	
Cr-Quinoline	:	
Fe-Quinoline	:	
Ni-Quinoline	:	

Zn-Quinoline	:	

Quinoline showed absorption at ultraviolet to violet region with the maximum wavelength in the ultraviolet region,λ_{max}= 214.39 nm. Mg-Quinoline has an absorption in blue to infrared light with a maximum wavelength in blue light area, λ_{max}= 470.57 nm. Ca-Quinoline has an absorption in the red to infrared regions with a maximum wavelength in the red light area, λ_{max}= 719.98 nm. Cr-Quinoline together with Ca-Quinoline has an absorption in the red to infrared region. It has a maximum withlength in infrared area, λ_{max}= 855.76 nm. Fe-Quinoline and Ni-Quinoline have absorption in infrared region with a maximum wavelength of each λ_{max}= 1764.39 nm andλ_{max}= 1325.20 nm. Actually, both of these compounds have also absorption in the red light up to pink light, but its intensity is very small so neglected in this study. The Zn-Quinoline has an absorption in the region of blue light to red light with a maximum wavelength in the blue light region,λ_{max}= 485.04 nm.

Photosensitivity of derivate compounds of quinoline shifted from the ultraviolet light into visible light region and infrared light region because of the conjugated metals. That work well in the visible light region is the conjugated metals Mg, Ca, Cr, and Zn although conjugation metals is partly also working in the infrared regions. While the rest of metal conjugate, is working in the infrared regions.

4. Conclusion

Characterization of the properties of organic semiconductor are made from quinoline and quinoline conjugated metals as the raw material of photo sensor indicate that band gap diminution occurs on the quinoline conjugated metal of Mg (Eg ~ 0.16 eV), Ca (Eg ~ 1.25 eV), Cr (Eg ~ 3.51 eV), Fe (Eg ~ 0.37 eV), Ni (Eg ~ 1.18 eV) dan Zn (Eg ~ 3.58 eV) than the bandgap of quinoline (Eg ~ 4.58 eV).Computational results are quite accurate because the infrared spectra are very consistent with the standard infrared spectra of the experimental result.

Photosensitivity of the quinoline conjugated metal seem to shift towards the maximum wavelength in the visible and infrared, ie Mg-quinoline (λ_{max}= 470.57 nm); Ca-quinoline (λ_{max}= 719.98 nm); Cr-quinoline (λ_{max}= 855.76 nm); Fe-quinoline (λ_{max}= 1764.39 nm); Ni-quinoline (λ_{max}= 1325.20 nm); dan Zn-quinoline (λ_{max}= 485.04 nm), compare quinolone photosensitivity that occurs in the ultraviolet region (λ_{max}= 214.39 nm).

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