

**LEMBAR
HASIL PENILAIAN SEJAWAT SEBIDANG ATAU PEER REVIEW
KARYA ILMIAH: PROSIDING**

Judul Publikasi Ilmiah (Artikel) : Ab initio computational study of -N-C and -O-C bonding formation : functional group modification reaction based chitosan

Jumlah Penulis : 6 orang

Status Pengusul : penulis anggota

Identitas Jurnal Ilmiah

a. Nama Jurnal Ilmiah: IOP Conference Series: Materials Science and Engineering

b. Nomor ISBN /ISSN : ISSN: 17578981

c. Volume, Nomor, Bulan, Tahun : Volume 349, Issue 1, 2 May 2018, Article number 012049

d. Penerbit : IOP Publishing

e. DOI artikel (jika ada) <https://doi.org/10.1088/1757-899X/349/1/012049>

f. Alamat web jurnal <http://iopscience.iop.org/issue/1757-899X/349/1>

g. Terindeks di SCOPUS (CiteScore is 0.53), Scimago journal Rank (H-index 24, SJR 0.192), Google Scholar, dll

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	Reviewer I	Reviewer II	
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b. Ruang lingkup dan kedalaman pembahasan (30%)	8	9	8,5
c. Kecukupan dan kemutakhiran data/informasi dan metodologi (30%)	8	9	8,5
d. Kelengkapan unsur dan kualitas penerbit (30%)	9	9	9
Total = (100%)	28	30	29
Nilai Pengusul = (40% x total)/5=	2,24	2,4	2,32

Reviewer 2

Prof. Dr. ref. nat Nuryono, M.S.
NIP. 196407141988111001

Unit kerja : Universitas Gadjah Mada Yogyakarta
Jabatan Fungsional : Guru Besar
Bidang ilmu : Kimia

Semarang,
Reviewer 1

Prof. Dr. Moh Djacri, ST, M.Eng
NIP 197102071995121001

Unit Kerja : Universitas Diponegoro Semarang
Jabatan Fungsional : Guru Besar
Bidang Ilmu : Teknik Kimia

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	(30)			
a. Kelengkapan unsur isi prosiding (10%)	3			3
b. Ruang lingkup dan kedalaman pembahasan (30%)	9			8
c. Kecukupan dan kemutakhiran data/informasi dan metodologi (30%)	9			8
d. Kelengkapan unsur dan kualitas penerbit (30%)	9			9
Total = (100 %)	30			28
Nilai Pengusul = (40% x 28)/5= 2.24				2.24

Catatan Penilaian artikel oleh Reviewer :

- Kesesuaian dan kelengkapan unsur isi artikel:**
Artikel sangat lengkap, dimana analisis tentang studi komputasi Ab initio pembentukan ikatan -N-C dan -O-C: reaksi modifikasi gugus fungsional berdasarkan kitosan disajikan dengan terperinci, disitasi dan dibahas. Topik dan materi sesuai dengan jurnal yang bersangkutan. Tata penulisan tersaji dengan sangat baik.
- Ruang lingkup dan kedalaman pembahasan:**
Artikel ini membahas tentang studi komputasi Ab initio pembentukan ikatan -N-C dan -O-C: reaksi modifikasi gugus fungsional berdasarkan kitosan. Berdasarkan studi tersebut diketahui bahwa sintesis N, O-CMC pertama terbentuk -O-CH₂COOH, kemudian berlanjut bentuk -NH-CH₂COOH. Informasi ini berharga untuk lebih mengoptimalkan kondisi reaksi Sintesis CMC. Beberapa rumus bangun dan struktur molekul yang ditampilkan perlu diberi referensi pendukung. Secara umum isi pembahasan cukup baik dan komprehensif, karena beberapa statemen penting ditunjang dengan referensi.
- Kecukupan dan kemutakhiran data/informasi dan metodologi:**
Referensi yang dicitasi dalam artikel ini ada 16 dimana 7 Baru (dalam 10 tahun terakhir). Nilai novelty/kebaruan artikel sangat baik. Analisa dan Metode disajikan dengan tahapan yang jelas, dan mudah diikuti.
- Kelengkapan unsur dan kualitas terbitan:**
Penerbit adalah IOP Publishing dan terindeks Scopus, SJR 0.19, H-index 24. Nilai similaritas artikel berdasarkan Turnitin hanya 4%, sehingga orisinalitas sangat baik.

Semarang, November 2019
Reviewer


Prof. Dr. Moh Djaeni, ST, M.Eng
NIP 197102071995121001
Unit Kerja : Universitas Diponegoro
Jabatan Fungsional : Guru Besar
Bidang Ilmu : Teknik Kimia

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	Internasional Bereputasi Berimpact factor (Prosiding)	Nasional Terakreditasi	Nasional	
	(30)			
a. Kelengkapan unsur isi prosiding (10%)	3			3
b. Ruang lingkup dan kedalaman pembahasan (30%)	9			9
c. Kecukupan dan kemutakhiran data/informasi dan metodologi (30%)	9			9
d. Kelengkapan unsur dan kualitas penerbit (30%)	9			9
Total = (100 %)	30			30

Nilai Pengusul = $(40\% \times 30)/5 = 2,4$

Catatan Penilaian artikel oleh Reviewer :

a. Kelengkapan unsur isi Jurnal:

Prosiding diterbitkan dalam IOP Conference Series: Materials Science and Engineering. Artikel yang diterbitkan dalam prosiding ini sangat lengkap, yaitu studi komputasi Ab initio pembentukan ikatan -N-C dan -O-C: reaksi modifikasi gugus fungsional berdasarkan kitosan. Tata penulisan cukup baik. Similaritas artikel berdasarkan Turnitin rendah (4%), orisinalitas sangat baik.

b. Ruang lingkup dan kedalaman pembahasan:

Ruang lingkup sesuai dengan Artikel ini membahas tentang studi komputasi Ab initio pembentukan ikatan -N-C dan -O-C: reaksi modifikasi gugus fungsional berdasarkan kitosan. Pembahasan diuraikan secara detail berdasarkan konsep/teori sah dan didukung dengan referensi.

c. Kecukupan dan kemutakhiran data/informasi dan metodologi:

Data yang disajikan sangat cukup dan layak untuk dipublikasikan di prosiding. Kemutakhiran cukup, referensi yang disitasi sebanyak 16, 10 (62%) terbit dalam 10 tahun terakhir dan 11 dari jurnal. Kebaruan artikel cukup baik. Metode dan prosedur disajikan dengan tahapan yang jelas untuk penelitian dengan kmputasi kimia.

d. Kelengkapan unsur dan kualitas Penerbit:

Penerbit adalah IOP Publishing (bereputasi) dan terindeks Scopus, SJR 0.19, H-index 24.

Yogyakarta, November 2019

Reviewer



Prof. Dr. Retnat Nuryono, M.S.

NIP. 196407141988111001

Bidang ilmu/Unit kerja :

Departemen Kimia pada Fakultas MIPA UGM Yogyakarta



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Volume 349, Issue 1, 2 May 2018, Article number 012049
12th Joint Conference on Chemistry, JCC 2017; Crystall Ballroom, Aston Hotel and Convention
Centre Semarang; Indonesia; 19 September 2017 through 20 September 2017; Code 136611

Ab initio computational study of -N-C and -O-C bonding formation : functional group modification reaction based chitosan (Conference Paper)

(Open Access)

Siahaan, P.^a ✉, Salimah, S.N.M.^a, Sipangkar, M.J.^a, Hudyanti, D.^a, Djunaidi, M.C.^a, Laksitorini, M.D.^b

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^aDepartment of Chemistry, Diponegoro University, Semarang, Indonesia

^bDepartment of Pharmaceutics, Faculty of Pharmacy, Gadjah Mada University, Sekip Utara, Yogyakarta, Indonesia

Abstract

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Chitosan application in pharmaceutics and cosmeceutics industries is limited by its solubility issue. Modification of -NH₂ and -OH functional groups of chitosan by adding carboxyl group has been shown to improve its solubility and application. Attempt to synthesize carboxymethyl chitosan (CMC) from monochloroacetic acid (MCAA) has been done prior this report. However no information is available whether -OH (-O-C bonding formation) or -NH₂ (-N-C bonding formation) is the preference for -CH₂COOH to attach. In the current study, the reaction mechanism between chitosan and MCAA reactants into carboxymethyl chitosan (CMC) was examined by computational approach. Dimer from of chitosan used as a molecular model in calculation All the molecular structure involved in the reaction mechanism was optimized by ab initio computational on the theory and basis set HF/6-31G(d,p). The results showed that the -N-C bonding formation via S_N2 than the -O-C bonding formation via S_N2 which have activation energy 469.437 kJ/mol and 533.219 kJ/mol respectively. However, the -O-C bonding formation more spontaneous than the -N-C bonding formation because ΔG the formation of O-CMC-2 reaction is more negative than ΔG of formation N-CMC-2 reaction is -4.353 kJ/mol and -1.095 kJ/mol respectively. The synthesis of N,O-CMC first forms -O-CH₂COOH, then continues to form -NH-CH₂COOH. This information is valuable to further optimize the reaction condition for CMC synthesis. © 2018 Institute of Physics Publishing. All rights reserved.

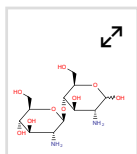
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Optimization of carboxymethyl chitosan synthesis using

Indexed keywords

Engineering controlled terms:

Activation energy Calculations Chitosan Computation theory Computational chemistry Dimers Solubility

Engineering uncontrolled terms

Ab initio Basis sets Carboxyl groups Carboxymethyl chitosan Computational approach Computational studies Modification reactions Reaction mechanism

Engineering main heading:

Chemical bonds

response surface methodology and desirability function

Bukzem, A.L. , Signini, R. , dos Santos, D.M. (2016) *International Journal of Biological Macromolecules*

Development of andrographolide-carboxymethyl chitosan nanoparticles: Characterization, in vitro release and in vivo antimalarial activity study | Andrografolid karboksimetil kitosan nanopartiküllerinin geliştirilmesi: Karakterizasyon, in vitro salım ve in vivo antimalaryal aktivite çalışması

Sari, R. , Widyawaruyanti, A. , Anindita, F.B.T. (2018) *Turkish Journal of Pharmaceutical Sciences*

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Thanks to Prof. Teruna J. Siahaan, Ph.D. (Pharmacy Department, University of Kansas, US), for the valuable direction and discussion of encapsulation and drug delivery systems. Thanks to the Directorate General of Higher Education. Last but not least Faculty of Science and Mathematics, which has funded this research through the Research Funding Scheme 2016.

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Publisher: Institute of Physics Publishing

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(2017) *Indonesian Journal of Chemistry*, 17 (2), pp. 291-300. Cited 6 times.
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Ab initio computational study of reaction mechanism of peptide bond formation on HF/6-31G(d,p) level ([Open Access](#))
(2017) *IOP Conference Series: Materials Science and Engineering*, 172 (1), art. no. 012040. Cited 2 times.
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doi: 10.1088/1757-899X/172/1/012040

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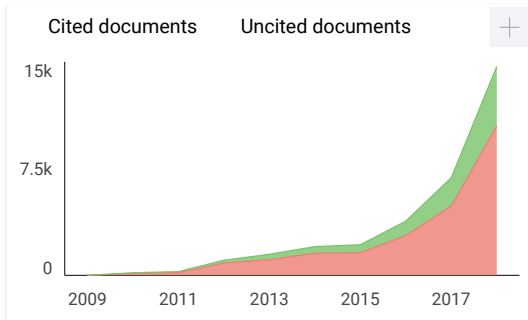
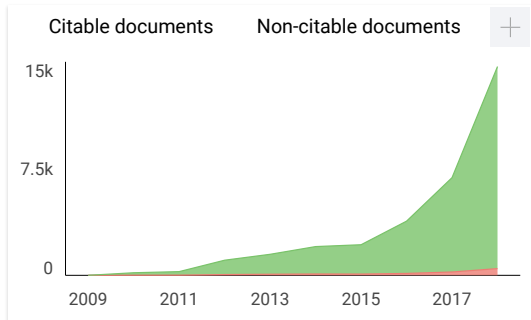
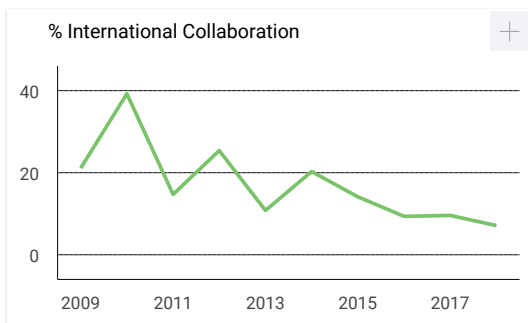
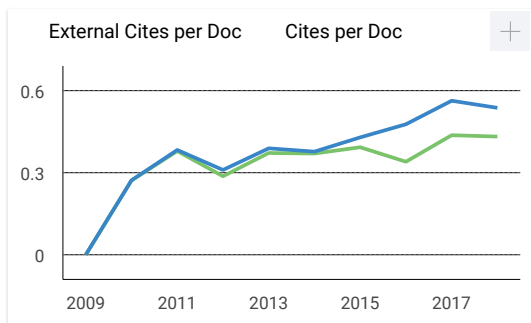
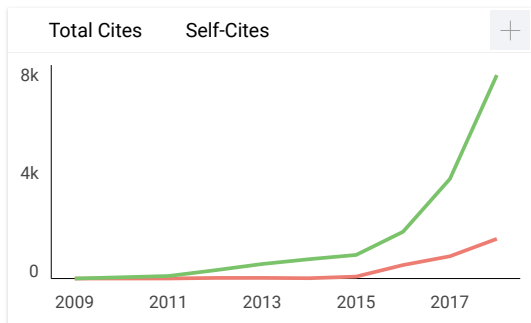
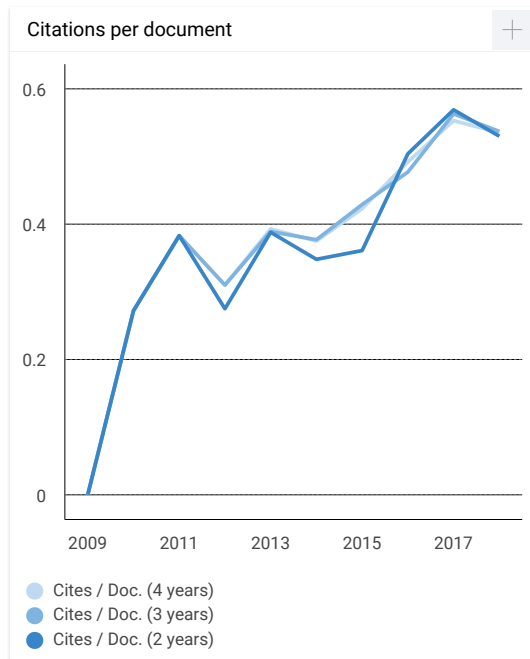
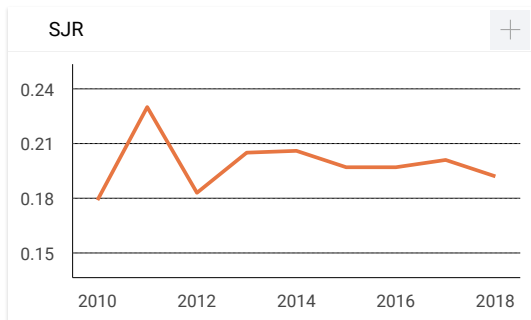
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Subject Area and Category	Engineering Engineering (miscellaneous) Materials Science Materials Science (miscellaneous)
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Publication type	Conferences and Proceedings
ISSN	17578981, 1757899X
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18 September 2017

18.30 – 21.00	Wecloming Dinner	Aston Hotel ballroom
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19 September 2017

07.00-08.15	Registration
08.15-08.35	Opening Ceremony
	Indonesia National Athem
	Welcoming Dance
08.35-08.40	Chairman speech Cepi Kurniawan, PhD
08.40-08.50	Welcoming from the head of department
08.50-09.00	Welcoming speech and opening the conference by the Dean Prof. Dr. Zaenuri M., S.E, M.Si, Akt.
09.00-09.20	Coffee Break
09.20-10.00	Prof. Guoping Chen Hybrid Scaffolds of Biodegradable Polymers and Biomimetic Matrices for Tissue Engineering Applications
	Chair: Sri Kadarwati, PhD
10.00-11.00	Prof. David Harding Designing Molecular Switches: A Molecular Magnetism Approach
	Prof. Hadariah Bahron Imines and Metals: Marriage Made in Heavens
	Chair: M. Alauhdin, PhD
11.00-12.00	Prof. Kasmadi Imam Kasmadi The Cultivation of Religious Characters in Chemical Science Learning
	Prof. Subramaniam Ramanathan
	Chair: Sri Kadarwati, PhD
12.00-13.00	Lunch Break
13.00-14.00	Prof. Ni Nyoman Tri Puspaningsih Strengthening The Academic Network on Bioresource Technology Research towards Green Industry
	Prof. Hajime Hirao Computationally Exploring Complex Molecular Systems
	Chair: M. Alauhdin, PhD

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JCC2017167

Golden Wattle (*Acacia pycnantha*) Flower: Is it Only Floral Emblem of Australia?

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Acacia pycnantha, commonly known as the golden wattle, belongs to the Fabaceae family. Typically, it grows from 3 to 8 meters in height, and is native to New South Wales, Victoria, and South Australia.¹ Despite their bright colourful flowers, and that it is regarded as Australia's national flower, there are no reports on the structures present within the flower. Therefore, we present the phytochemical constituents in the flower, as well as correlations to their biological activities. The crude methanol were subjected to liquid-liquid extraction to provide hexane, ethyl acetate, and residual fractions. RP-HPLC profiles of both the ethyl acetate and residual fractions produced similar profiles. Thus, the ethyl acetate fraction was selected, and subjected to HPLC separation. Utilising the optimized preparative HPLC method, eight known compounds were isolated, and identified as (2*S*)-isohemiphloin (**1**), (2*S*)-naringenin-5-*O*-glucoside (**2**), kaempferol 3-rutinoside (**3**), quercetin 3-glucoside (**4**), myricetin 3-rhamnoidise (**5**), kaempferol-3-rhamnoside (**6**), isosalipurposide (**7**), naringenin (**8**) by comparison of their spectral data with those reported in the literature. Furthermore, the extract and all isolated compounds were assessed for antibacterial activities against several human pathogenic bacteria by Hit-confirmation method with various results.

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JCC2017179

The Effect of Mangoosteen Extract (*Gracinia Mangostana L.*) on Synthesis of Ag_3PO_4 Photocatalyst

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Today, silver orthophosphate has been developed as photocatalyst for dye removal under visible light irradiation due to owing small-band gap energy of ~ 2.42 eV (1), strong photooxidative (2,3) and high quantum yield (3). The morphology and composites design have been applied to improve this photocatalyst. Morphology of saddle-like tetrahedron (4), coral-like microspheres (5), branched Ag_3PO_4 crystal with porous structure (6) and truncated tetragonal bipyramids (7) had improved the photocatalytic activity.

The big challenge of Ag_3PO_4 development is improvement the surface area and stability of photoreaction. The photocatalytic activity of Ag_3PO_4 is strongly affected by the size and surface area (8). Previous work showed that the synthesis of Ag_3PO_4 using PEG and PVP increased the specific surface area and enhanced the photocatalytic activity (9). Most of the preparation of Ag_3PO_4 catalyst using co-precipitation method resulted in low surface area. The poor performance of Ag_3PO_4 is attributed to the large particle size, which results in a low surface area, and thus low photocatalytic activity. Therefore, the development of the Ag_3PO_4 synthesis to design the small particle size is very important.

Herein, the Ag_3PO_4 prepared under mangoosteen (*Gracinia mangostana L.*) extract addition to the starting solution of AgNO_3 and $\text{Na}_2\text{HPO}_4 \cdot 12\text{H}_2\text{O}$ could significantly decrease the particle size and increase the crystalline of Ag_3PO_4 . This result enhances the photocatalytic activity. The mangoosteen extract solution of 0%, 1% and 1.5% were applied to producing the Ag_3PO_4 using the starting material of AgNO_3 and $\text{Na}_2\text{HPO}_4 \cdot 12\text{H}_2\text{O}$. Samples were characterized using x-ray diffraction and scanning electron microscopy. Photocatalytic activities were evaluated using Rhodamine B photooxidation under blue light irradiation. The mangoosteen extract addition greatly decreases the particle size and increases the crystallinity of Ag_3PO_4 which significantly enhances the photocatalytic activity.

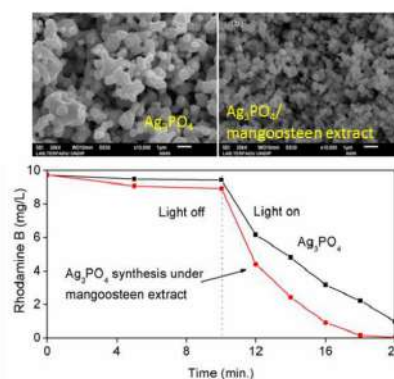


Fig. 1 Morphology and Catalytic Activity

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JCC2017212

Supramolecular Assembly of Group 11 Phosphorescent Metal Complexes for Chemosensors of Alcohol Derivatives

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Transition metal complexes with phosphorescent properties have been utilized as chemical sensors (chemosensors) with high sensing capability for sensing different kinds of volatile organic compounds (VOCs). However, there is no study on molecular design of metal complexes toward high sensing capability. Therefore, by using 4-(3,5-dimethoxybenzyl)-3,5-dimethyl pyrazole ligand¹⁾ (**1e**) and group 11 metal ions (Cu(I), Ag(I), Au(I)), we report the systematic study on vapochromic sensing of VOCs such as alcohol derivatives using phosphorescent trinuclear pyrazolate complexes with supramolecular assembly of a weak intermolecular metal-metal interactions. Previously, the resulting trinuclear copper(I) 4-(3,5-dimethoxybenzyl)-3,5-dimethyl pyrazolate complex **2e(Cu)** revealed positive response to ethanol vapors by blue-shifting its emission band from 616 to 555 nm and emitting bright orange to green where the original intensity can be easily recovered and then reused without external stimuli.²⁾ Moreover, **2e(Cu)** still showed the best performance for chemosensor of ethanol vapors compared to the same complexes synthesized from different side-chains at the pyrazole rings such as non-side chain, 3,5-dimethyl, 3,5-bis(trifluoromethyl), and 3,5-diphenyl pyrazole ligands.³⁾ In this lecture, we particularly discuss the sensing capability of group 11 metal ions with the same ligand **1e**. Upon excitation at 284, the resulting complexes showed emission bands with a peak centered at 616, 473 and 612 nm for **2e(Cu)**, **2e(Ag)** and **2e(Au)**, respectively. Comparing to **2e(Cu)** with shorter metal-metal distance for sensing ethanol vapors in 5 mins, **2e(Au)** gave shifting from its emission band centered at 612 to 587 nm with $\Delta\lambda$ of 25 nm and color changes from red-orange to light green-orange. This blue-shifting was 41% compared to **2e(Cu)** with the same exposure time while the reusability testing required the presence of external stimuli. On the other hands, **2e(Ag)** with longer metal-metal distance showed quenching in its original emission intensity at 473 nm in 40% with color changes from dark green to less emissive. These results demonstrate that shifting phenomenon in **2e(Cu)** with the shorter metal-metal distance compared to **2e(Au)** from the same ligand is due to a weak intermolecular hydrogen bonding interaction of O atom at the methoxy of the benzyl ring with the OH of the vapors at the outside of the molecules. Such sensing phenomenon cannot be achieved for the detection of propanol, butanol, pentanol and hexanol vapors with decreasing in the performance to 37%, 28%, 23% and 18%, respectively, indicating suitable molecular design of ligand and metal ion in pyrazolate complex as chemosensor **2e(Cu)** for sensing ethanol vapors.

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JCC2017306

**Effect of Potentials and Electric Charges Copper and Indium
Depositions to The Photocurrent Responses of CuInS₂ Thin Film
Fabricated By Stack Electrodeposition Followed by Sulfurization**

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Effect of potentials and electric charges copper and indium depositions to the photocurrent responses of CuInS₂ thin film fabricated by electrodeposition followed by sulfurization were investigated. The characterization and elemental compositions of as-deposited Cu/In and CuInS₂ thin films used X-RD and EDAX. Photocurrent responses of the obtained CuInS₂ thin films were analyzed by linear sweep voltammograms (LSVs) in europium solution under chopped irradiation. Photocurrent responses showed that fabricated CuInS₂ thin films had *p*-type photoresponses. Improving potentials and electric charges reduced the photocurrent responses of the semiconductor films, although from XRD and EDAX data had no significant different.



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