SYMPOSIUM

Environmental Chemistry (ENV)

The influence of Hibiscus tiliaceus extract in zinc oxide properties and its performance on simultaneous removal of chromium (VI) and methylene blue

Riki Subagyo[1], Ceisar Andria Putra[, Siyam Matina [2,3], Saepurahman [3] Yuly Kusumawati[*1]

[1]*Department of Chemistry, Faculty of Science and Data Analytics, Institut Teknologi Sepuluh Nopember, Kampus ITS Keputih, 60111, Sukolilo, Surabaya, Indonesia*
[2]*Department of Chemistry, Faculty of Mathematics and Natural Sciences, Universitas Negeri Semarang. Gd. D6 Kampus Sekaran Gunungpati, Semarang, Indonesia 50229*
[3]*Research Center for Chemistry, National Research and Innovation Agency (BRIN), Gd. 452 Kawasan Puspiptek Serpong, Tangerang Selatan 15314, Indonesia*

[*]Corresponding email: y_kusumawati@chem.its.ac.id

ABSTRACT

Here, we reported the influence of Hibiscus tiliaceus extract in the formation of zinc oxide (ZnO) using polyol methods. The Hibiscus tiliaceus extract is utilized to change the water in hydrolysis ratio of Zn^{2+}/water. The diffraction pattern results confirmed that ZnO was formed using water (ZnO-w) or Hibiscus tiliaceus extract (ZnO-e). The enlarged XRD peaks of (101) plane showed the shift in peaks with the addition of Hibiscus tiliaceus extract, associated to the variant in residual strain developed in the crystal lattice. Fourier transform infrared spectra of synthesized ZnO exhibit the similar spectra at wavenumber of 3430 cm^{-1}, 1650 cm^{-1}, 1550 cm^{-1} and 600–400 cm^{-1}. The use of Hibiscus tiliaceus extracts leads to the formation of ZnO with a larger particle size compared to the use of water, which was in agreement with diffraction pattern. Therefore, the usage of Hibiscus tiliaceus extracts alter the bandgap energy in visible range. An excellent performance of ZnO-w in simultaneous removal of chromium and methylene blue compared with ZnO-e, revealing that the synergistic of particle size and band gap energy is crucial factor in photo-removal process.

The Influence of Storage Solution on Swelling Degree of Agarose Crosslinked with Oxalic Acid as Diffusion Layer for DGT

Layta Dinira[*1], Barlah Rumhayati[1], Ulfa Andayani[1], Diah Mardiana[1]

[1] *Dept. of Chemistry, Brawijaya University, Malang*

[*]Corresponding email: laytadinira1@student.ub.ac.id

ABSTRACT

The Diffusive Gradient in Thin Films (DGT) technique has been widely used as passive sampling in waters. The analyte will diffuse through the diffusive gel and then retain in the binding layer. Agarose can be used instead of polyacrylamide as diffusive gels. The agarose pores need to be minimized by cross-linking the agarose with oxalic acid. The gel was prepared by adding oxalic acid solution to agarose solution at 60 $^{\circ}$C. The solution was stirred and then immediately pipetted into the mold. The mold containing the mixed solution was heated in an oven for 15 minutes at a casting temperature of 40, 50, and 60 $^{\circ}$C. The gel was washed with distilled water and then cut into rounds. The gel was immersed for one, two, three, and up to 24 hours in a storage solution of pH 4 – 8. The mass, diameter, and thickness of the initial gel and each immersion time were measured. The round gel that was made at 40 $^{\circ}$C was also immersed for one, two, three, and up to 24 hours in a NaNO$_3$ storage solution of 1 x 10^{-4} – 0.75 M. The results showed that rather than the gel made at 50 and 60 $^{\circ}$C, the swelling degree of agarose gel cross-linked with oxalic acid during 24-hour immersion time made at 40 $^{\circ}$C is not affected by the pH of the storage solution. 0.0001 – 0.1 M NaNO$_3$ solution can be used to store agarose crosslinked with oxalic acid made at 40 $^{\circ}$C.

FLOW INJECTION ANALYSIS (FIA) SYSTEM FOR CONTINUOUS MONITORING OF WATER QUALITY

Adam Wiryawan

Department of Chemistry, Brawijaya University

*Corresponding email: adammipa@ub.ac.id

ABSTRACT

Development of industrial areas must be followed by increased monitoring of industrial wastewater and water systems.. One method for continuous monitoring of process and product water quality is flow injection analysis (FIA). An FIA method does not need to mix the reagents and sample manually as in methods based on conventional spectrophotometry and colorimetry; they are delivered by peristaltic pump to the manifold, and after mixing, they go into the flow cell. The parameters that can be determined by FIA are nitrite, nitrate, ammonia, phosphate, silica, arsenic, and mercury, etc. The simple flow injection analyzer consists of : (1) a pump used to propel the carrier stream through a tube; (2) an injection port through which a well-defined volume of sample solution is injected into the carrier stream in a very reproducible manner; (3) a reaction coil or manifold, in which the sample zone disperses and reacts with component from carrier stream to form a species; and (4) a flow-through detector cell (FC) that allows continuous measurement. Key word : FIA, continuous, monitoring, water quality

Process of Optimizing CO_2 Gas Absorption by Zeolite

Andi Nafis An Naafi[*1], Rachmat Triandi Tjahjanto[2], Yuniar Ponco Prananto[3]

[1]*Dept. of Chemistry, Brawijaya University, Malang*

[*]Corresponding email: andinafisan@gmail.com

ABSTRACT

Zeolite is a natural material that belongs to the aluminosilicate group with porous and hollow characteristics and channels. These characteristics can determine its usefulness as a material for adsorption or catalyst processes. The advantages of zeolite as an adsorbent for the adsorption process are environmentally friendly, low energy capacity, inexpensive, and easy to apply. Several researchers have carried out the adsorption process by varying the type of adsorbent, the amount of adsorbent, temperature, pressure, flow rate, absorption time, and the shape of the column used. However, the adsorption process is still being studied by researchers to obtain more optimal and better results than previous studies. In this study, the adsorption process used NaOH solution with a concentration of 0.2 M, natural zeolite, and activated zeolite. The tools used in the adsorption process are a column with a capacity of 25 grams of adsorbent and two flowmeters. The adsorption process was carried out for 1 minute to 8 minutes with a gas flow rate of 1 L/minute with 25 grams of zeolite and 0.2 M NaOH solution. Analysis of CO_2 levels was obtained through the titration method using NaOH solution that absorbs CO_2 gas. Optimal absorption results were obtained from activated zeolite (NaOH 1.0 M) when CO_2 was absorbed for 5 minutes with a percentage of 99.84% and decreased after that. Thus, the column filled with active zeolite can improve the adsorption ability and obtain a higher optimization rate. *Keywords: Zeolite, activation, adsorption, CO_2*

SYMPOSIUM

Catalysts and Catalysis (CAT)

Palm Oil Epoxidation by V2O5/Al2O3

Eunike Kartika Salduna[*1], Yessi Permana[2]

[1,2] *Chemistry, Faculty of Mathematics and Natural Science, Bandung, Indonesia*

[*]Corresponding email: eunikekartikasalduna@gmail.com

ABSTRACT

European countries recently reduced the use of phthalates as plasticizers because of toxicity. Vegetable oil epoxides were reported as alternative plasticizers with nontoxic and benign properties. Palm oil epoxide (epoxidized palm oil or EPO) shows and is produced by oxidizing triglyceride olefins using H2O2 and acids. However, the process releases heat uncontrollably, corrosive, and decrease the selectivity because of further hydrolysis of epoxide rings. The oxidation reaction of palm oil in this study used tertiary-butyl hydrogen peroxide or TBHP as an oxidizing agent, assisted by V2O5/γ-Al2O3 (1 : 10 mol). The support of γ-Al2O3 was chosen because it may deposit vanadia while providing ease process of catalyst regenerations. The regeneration of unsupported-V2O5 from palm oil is relatively difficult. Synthesis of V2O5/γ-Al2O3 is carried out by dropwise impregnation of alumina by a solution of VO(acac)2 complex followed by heating at 100 oC (2 h) and calcination at 500 oC (5 h). Catalytic reaction tests were also conducted with various types of 1st raw transition metal oxides, impregnated on alumina (Cr2O5, CuO, Fe2O3, NiO) to evaluate the oxide character. The observation showed excellent epoxidation on V2O5/γ-Al2O3 employmentresults compared to other oxides. Optimized reaction conditions were achieved at 80 oC, 7 h, 0.5 mol% of vanadium upon olefins, and 3.5 mol eq. of TBHP. A longer reaction indicated the opening of epoxide rings. A kinetics study showed that the reaction was a pseudo-2nd order with an activation energy (Ea) of 27 kJ.mol-1, turn over number (TON) of 138 and turn over frequency (TOF) of 20 h-1. Such an activation energy is lower than the reported uncatalyzed-reaction (Ea of 91 kJ.mol-1). The catalytic study described free Gibbs energy (ΔG‡) 90 kJ.mol-1, entropy (ΔS‡) -188 J.mol-1.K-1 , and enthalpy (ΔH‡) 24 kJ.mol-1. Recycling of V2O5/γ-Al2O3 catalysts was carried out by ethanol rinsing and drying at 80 oC (1 h). Recycled-catalyst gave relatively good epoxidized oil (up to 75% PO conversion). Epoxidation of waste-cooking oil (WCO) resulted in epoxidized WCO of 50% PO conversion . Keywords: Palm oil, epoxidation, V2O5/γ-Al2O3

Gasoline-Range Hydrocarbon Production from Hydrocracking of LDPE Plastic Waste Utilizing Nickel-Promoted Sulfated Nanozirconia Catalyst

Amalia Kurnia Amin[1,2], Wega Trisunaryanti[2], Karna Wijaya[*2]

[1]*Research Center for Chemistry, National Research and Innovation Agency, South Tangerang 15314, Indonesia*
[2]*Department of Chemistry, Universitas Gadjah Mada, Yogyakarta 55281, Indonesia*

[*]Corresponding email: karnawijaya@ugm.ac.id

ABSTRACT

Single-used LDPE plastic waste was converted to liquid fuels-like through hydrocracking over Ni/ZrO_2-SO_4 under various operating conditions. Optimizing temperature reaction and feed-to-catalyst ratio were assessed to obtain the maximum gasoline fraction. The highest liquid product (65.91 wt.%) that contains a high fraction of gasoline (83.22%) was yielded from catalytic hydrocracking at 250 °C for 60 min with a feed-to-catalyst ratio of 100/1. In comparison to ZrO_2 and SZ, the 1.5NiSZ-R catalyst showed comparatively high catalytic activity, selectivity, and good recyclability for producing gasoline up to four cycles.

Hydrogenation and Hydrogenolysis of Furfural using Zr-MOFs

Melana Daniela Nguru[1], Hilda Nuraulia[1], Yessi Permana[*1]

[1]*Dept. of Chemistry, Bandung Institute of Technology, Bandung*

[*]Corresponding email: yessi@itb.ac.id

ABSTRACT

Furfural (FAL) is one of the biomass derivatives that plays a key role because it can be further processed to produce other compounds that are widely used in food, medicine, resin, plastic, and other industries. Hydrogenation of FAL mainly produces furfuryl alcohol (FOL) which is used in polymer and coating industries. Further hydrogenation and hydrogenolysis of FOL will produce tetrahydrofurfuryl alcohol (THFA), which is widely used as a green solvent in industry, and 1,2-pentanediol (1,2-PeD), a preservative in cosmetics and disinfectants. In this study, various zirconium(IV) metal-organic frameworks (Zr-MOFs) were used as the catalyst in the furfural hydrogenation and hydrogenolysis using ethanol and isopropyl alcohol as the hydrogen sources. The synthesized Zr-MOFs were characterized using powder XRD and FTIR. The conversion of FAL was observed using gas chromatography (GC). Multiple experimental conditions such as temperatures and reaction time were tested and the yield was analyzed to obtain the optimum condition to produce THFA and 1,2-PeD. We found that the reaction of furfural in 2-propanol at 160°C for 5h by MOF-808 and vanadyl@MOF-808 gave respectively 16.4% and 82% of 1,2-PeD, while the same reaction in ethanol gave respectively 68.1% and 58.6% of THFA. Keywords: furfural; furfuryl alcohol; Zr-MOFs; 1,2-pentanediol, tetrahydrofurfuryl alcohol

Selective Synthesis of 1,2-Pentanediols from Furfuryl Alcohol by $CoWO_4$

Siti Hartinah Qurbayni[1], Husni Wahyu Wijaya[2], Ubed Sonai Fahruddin Arrozi[2], Yessi Permana[*1]

[1]*Inorganic and Physical Chemistry Research Division, Faculty of Mathematics and Natural Sciences, Institut Teknologi Bandung, Bandung*
[2]*Department of Chemistry, Faculty of Mathematics and Sciences, State University of Malang, Malang*

[*]Corresponding email: yessi@itb.ac.id

ABSTRACT

Abstract Furfuryl alcohol (FOL) is a biomass derivative used in polymer and pharmaceutical industries. Hydrogenation and hydrogenolysis of FOL were reported to give 1,2-pentanediol and 1,5-pentanediol in pressurized hydrogen by platinum group metals (Ru, Pd, and Pt). Such a reaction was commonly facilitated by pressurized hydrogen. Cobalt tungstate ($CoWO_4$) was evaluated here as a catalyst with hydrogen sources of alcohol. $CoWO_4$ was synthesized hydrothermally at relatively lower temperature (<160 °C) and shorter time (<10 hours) compared to previously reported procedure (180-200 °C, 15-24 hours). This work also evaluated the amorphous phase of $CoWO_4$. The catalytic activity of $CoWO_4$ in crystalline and amorphous phases were observed in the hydrogenolysis of FOL in the absence of pressurized hydrogen. The freshly prepared $CoWO_4$ was characterized using PXRD, FTIR, and EDX. The conversion of FOL and products were observed by gas chromatography (GC) and 1NMR. We found that the reaction of FOL in 2-propanol at 160 °C for 7 h by amorphous $CoWO_4$ resulted in 1,2-pentanediol (67%), while the same reaction in ethanol gave 54% of tetrahydrofurfuryl alcohol (THFA). Keywords: furfuryl alcohol; $CoWO_4$; 1,2-pentanediol; tetrahydrofurfuryl alcohol

Comparative Study of Low-Grade Crude Coconut Oil Esterification over SO_4/ZrO_2 and SO_4/TiO_2 Catalysts

Karna Wijaya[*1], Latifah Hauli[2], Yufinta Candrasasi[1], Edhita Rahmawati Fitri[1], Prisnu Fadilah Prabani[1]

[1]*Department of Chemistry, Gadjah Mada University, Yogyakarta*
[2]*Research Center for Chemistry, National Research and Innovation Agency (BRIN), South Tangerang*

[*]Corresponding email: karnawijaya@ugm.ac.id

ABSTRACT

The esterification reaction has been performed using SO_4/ZrO_2 (SZ) and SO_4/TiO_2 (ST) catalysts. SZ and ST catalysts were synthesized using the wet impregnation method. SZ and ST catalysts were characterized by FTIR before and after the acidity test and then applied to the esterification step. The esterification process was carried out with variations in the weight of SZ and ST catalysts (1, 3, 5, and 7%) from the total weight of oil and methanol, variations in reaction time (30, 60, 90, 120, 150, and 180 minutes), and variations in reaction temperature (35, 45, 55, and 65 °C). FTIR and GCMS characterized the esterified oil. The optimum conditions of the esterification process were obtained at 5% weight of SZ and ST catalysts, a reaction time of 150 minutes, and a temperature of 55 °C for SZ and ST catalysts. The SZ catalyst obtained a reduction percentage in FFA content of 65.80%, while the ST catalyst was 72.05%.

SYMPOSIUM

Advances in Nanomaterials (NNO)

EXTRACTION OF LOW RANK COAL BASED ON GRAPHENE (Gs) AND GRAPHENE QUANTUM DOTS (GQDs) USING REPEATABLE ULTRASONICATION TECHNIQUE

Vivi Purwandari[*12], Isnaeni [2], Penny Oktaviani [3], Fatimah [3]

[1] *Chemistry Dept, Faculty of Science, Technology and Information, Sari Mutiara Indonesia University, Medan*
[2] *Research Center for Photonics, National Research and Innovation Agency, Indonesia*
[3] *Pusat Sumber Daya Mineral Batubara dan Panas Bumi*
Jl. Soekarno Hatta no 444 Bandung

[*]Corresponding email: drvivipurwandari@gmail.com

ABSTRACT

The nanocrystal structures present in coal during the coalification process are ideal precursors for nanocarbons such as graphene (Gs) and graphene quantum dots (GQDs). In this study, we report an easy and environmentally friendly method for the preparation of Gs and GQD using the One-Step Ultrasonication method of lignite coal in Isopropyl alcohol. This study uses 2 types of coal, namely lignite and subbituminous. The Photoluminescence (PL) test showed that both lignite coal samples emit a reddish-yellow fluorescence and subbituminous emit blue fluorescence under ultraviolet light. TEM analysis confirmed the presence of a mixture of nanocarbons, both graphene layers and graphene quantum dots. It was concluded that graphene sheets (Gs), graphene quantum dots (GQDs) could be extracted from low grade coal only by one step ultrasonication method. These fluorescence carbon nanostructures can be applied to optoelectronic devices or permanent energy devices such as supercapacitors.

Synthesis of Mesoporous Silica SBA-15 using the Ultrasonic Assisted-Sol Gel Method and Its Characterizations

RR Dirgarini Subagyono[*], Siti Sarah, Veliyana Londong Allo

Physical Chemistry Laboratory, Chemistry Department, Mulawarman University, East Kalimantan, Indonesia

[*]Corresponding email: dirgarini@fmipa.unmul.ac.id

ABSTRACT

The synthesis of mesoporous silica material SBA-15 using the Ultrasonic Assisted Sol-gel Method has been conducted. The synthesis of SBA-15 was carried out by varying the sonication time, the type of acid and the template removal method. The mesoporous silica material was characterized by N_2 adsorption/desorption Analysis, Small Angle X-Ray Diffraction (SAXRD), Scanning Electron Microscopy (SEM), and Fourier Transform Infrared (FTIR). Analysis of the hydroxyl group content on the silica surface was carried out using the Thermogravimetric Analysis (TGA). The results showed that the length of sonication time, type of solvent and template removal method affected the surface area, pore volume, pore diameter, lattice spacing (d100) and unit cell parameters, as well as morphology and hydroxyl group content of the resulting SBA-15 material. SBA-15 material resulted from the calcination method for template removal has a surface area of 620-770 m^2/g, a pore volume of 1.06-1.21 cm^3/g and a pore diameter of 6.3-6.8 nm, while the SBA-15 material with the addition of H_2O_2 for template removal has a surface area of 177-195 m^2/g, a pore volume of 6.9 cm^3/g and a pore diameter of 14-15 nm. The SAXRD pattern of SBA-15 showed three distinctive peaks with Miller indeces of 100, 110 and 200 respectively. The morphology of the SBA-15 material was macaroni-like and in aggregate form. Infrared spectra of SBA-15 showed the presence of functional groups, namely Si-O-Si, Si-OH and –OH. The SBA-15 material produced by the calcination method has a lower hydroxyl group content than that by the addition of H_2O_2.

Synthesis and characterization of cellulose acetate/ZIF-8/graphene oxide-based mixed matrix membranes

Putu Doddy Sutrisna[*1], Verdianto Indra Wijaya Sutama Putra[1], Putu Dhiyo Dharmayoga Denaswara[1]

[1] *Dept. of Chemical Engineering, University of Surabaya (UBAYA), Surabaya, Indonesia*

[*]Corresponding email: pudod@staff.ubaya.ac.id

ABSTRACT

Membrane technology is one of waste water treatment methods that has a potential to provide high removal at low cost. However, the conventional membrane still has a low rejection, whereas when rejection is increased, it will result in decreased flux. Therefore, Mixed Matrix Membranes (MMMs) were developed with a combination of Zeolitic Imidazolate Framework 8 (ZIF-8) and Graphene Oxide (GO) as the fillers which have the potential to increase permselectivity as well as membrane permeability. This research was conducted to study about the effect of ZIF-8 and GO composition as the fillers on cellulose acetate-based MMMs on their morphological and chemical structures using SEM, FTIR, and XRD, in addition the effect to membrane performance by testing the flux and rejection parameters on membranes. The results of SEM analysis showed that the pore size of MMMs were in the range 0.1 – 0,5 µm and increasing the amount of filler tends to cause particles agglomeration. The FTIR results did not show a significant change with the addition of GO in the %transmittance obtained. XRD results showed an increasing peak when GO was added up to 0.6%wt, although decreased at 1%wt. At the membrane performance test, increasing the concentration of ZIF-8 could increase the rejection, however it would decrease the flux. By adding GO, the flux could be increased, but also indirectly decreasing the rejection with an insignificant value. Increasing the concentration of methylene blue used has an impact on decreasing both flux and rejection.

SYMPOSIUM

Computational Chemistry (COM)

Selectivity Study of Derivate 15-Crown-5 for Heavy Metals Extraction

Achmad Wisnu Adi Riyanto, Lalu Rudyat Telly Savalas, Saprizal Hadisaputra[*]

Chemistry Education Division, Faculty of Teachers Training and Education, University of Mataram. Indonesia

[*]Corresponding email: rizal@unram.ac.id

ABSTRACT

The capability of benzo-15-crown-5 ether to form complexes with some heavy metals cation (Cd^{2+}, Hg^{2+}, and Pb^{2+}) have been investigated by density functional theory method (DFT) using Gaussian system. The DFT calculations were performed by 6-311G(d,p) with LANL2DZ ECP basis set at the B3LYP level of theory. The interaction energies were used to evaluate the metal binding capability of the crown ethers. The influence of adding substituents was also studied. The result of these calculation showed that the number of ion charge transfer is proportion with the increasing of the interaction energy, furthermore the existence of the electron donating group (EDG) affected the crown ether's ability to bind heavy metals cation. In addition, based on the extraction interaction energy, charge transfer, and the electron distribution at the HOMO-LUMO orbitals can be concluded that the selectivity order of 15-crown-5 derivate is $Cd^{2+} > Hg^{2+} > Pb^{2+}$.

Anti-Breast Cancer Activities from the Sea Fan (Gorgonia mariae): Pharmacophore Screening and in silico Molecular Docking Study

Faruk Jayanto Kelutur[*1]

[1]*Study Program of Pharmacy, Institute of Health Science Salsabila Serang, Banten*

[*]Corresponding email: farukjayantokelutur@ymail.com

ABSTRACT

Sea fan, a type of gorgonian coral originating from Maluku, Indonesia which local people have used as medicinal ingredients for generations. Gorgonian has anti-inflammatory, anti-cancer, analgesic, gastroprotective, anti-viral, anti-bacterial, and anti-fouling activities with secondary metabolites steroid found in abundance. Steroid significantly inhibits the estrogen receptor that triggers breast cancer. However, the activity of these metabolites on sea fan has not been studied. Determination of specific receptor with Swiss Target Prediction, then the interaction ability of steroid of sea fan from binding pocket using Ligand Scout 4.4.3, while ligand-protein interaction with Autodock Tools 1.5.6. Based on the target prediction results, the steroid of sea fan significantly acts on the target class of estrogen receptor alpha (ER-α). Pharmacophore identification shows that steroid components can act as lead compounds to ER-α with pharmacophore fit scores (%) is 44.47 (dinosterol), 38.72 (4,24-dimethyl cholestanol), 38.71 (4,24-dimethyl 22-dehydro cholestanol and 4-methyl 24-methylene cholestanol), as well as 38.70 (4,24-dimethyl cholesta 7,22-dien-3ß-ol), respectively. In silico molecular docking obtained free energy of binding (ΔG, kcal/mol) and inhibition constant (Ki, nM), namely -12.14; 1.26 (4,24-dimethyl 22-dehydro cholestanol), -11.05; 7.97 (4,24-dimethyl cholesta 7,22-dien-3ß-ol), and -11.00; 8.57 (4,24-dimethyl cholestanol), respectively. The molecular docking mentioned value was much higher than the reference ligand, tamoxifen (-10.44 kcal/mol; 22.12 nM). So, it can be concluded that steroids (4,24-dimethyl 22-dehydro cholestanol; 4,24-dimethyl cholesta 7,22-dien-3ß-ol; and 4,24-dimethyl cholestanol) from the sea fan have potential as inhibitor ER-α. Keywords: sea fan, breast cancer, pharmacophore, in silico

COM/O-003

Deciphering the mechanism of the nickel-catalyzed catalytic transfer hydrogenation of furfural to furfuryl alcohol

Nova Pratiwi Indriyani[1], Azi Ibnu Sulistia[1], I Made Arcana[1], Muhamad Abdulkadir Martorprawiro[1], Aditya Wibawa Sakti[2], Yessi Permana[*1]

[1]*Inorganic and Physical Chemistry Research Division, Faculty of Mathematics and Natural Sciences, Institut Teknologi Bandung*
[2]*School of Advanced Science and Engineering, Global Center for Science and Engineering, Departement of Chemistry and Biochemistry, Waseda University*

[*]Corresponding email: yessi@itb.ac.id

ABSTRACT

Current methods for catalytic hydrogenation of furfural valorization are limited by their use of noble metals such as Ru, Pd, Pt, Ir and Au as catalysts at high pressures of H_2 (up to 100 bar). In this work, the air stable and inexpensive Ni(II)-phosphine complex, $NiCl_2(PPh_3)_2$, was explored as a catalytic transfer hydrogenation precursor in furfural valorization in the presence of Zn as a reduction agent as well as ethanol as hydrogen transfer agent, to produce furfuryl alcohol under relatively mild conditions (7 h, 160 $^{\circ}$C). Experimental studies suggest the rule of Ni(0) phosphine complex as an active species in this catalytic reaction. Quantum chemistry calculations were performed at density-functional theory level by employing MN15L functional to decipher the reaction mechanism of the reduction of furfural to furfuryl alcohol. The present work has revealed that the reaction proceeds through the following five essential elementary steps: (i) the oxidative addition of ethanol to the nickel catalyst, (ii) the β-H-elimination to form a nickel-hydride complex, (iii) the furfural coordination to nickel complex, (iv) the β-H-elimination from the hydride to the carbonyl oxygen of furfural, and (v) the reductive elimination to form the furfuryl alcohol. Based on the calculated free energy barriers, the first step of hydrogen transfer from nickel-hydride to the carbonyl oxygen of furfural moiety is the rate determining step (RDS) of the overall reaction. The catalytic efficiency was investigated by calculating the free energy barrier at the RDS for various type of ligands on nickel complex, namely, triphenylphosphine, triphenylphosphite, and tri-p-tolylphosphine. Furthermore, the Lewis acidity has been determined via the electrostatic potential charge calculations.

Docking of Heparin 2S and 2SNS with ^{2}S$_{0}$ IDS Conformation Oligomer on FGFR1-FGF2 Ligand-Receptor Terner Complex

Himmatul Barroroh[*][1,2] Nilna R. Maulidia[1] Lukman Hakim[2] Anna Safitri[2] and Widodo Widodo[2]

[1]*Faculty of Science and Technology UIN Maulana Malik Ibrahim Malang, Jl. Gajayana No.50 Malang, East Java, Indonesia, 65144.*
[2]*Faculty of Mathematics and Natural Sciences Brawijaya University, Jl. Veteran Malang, East Java, Indonesia, 65144*

[*]Corresponding email: himmatul.b@kim.uin-malang.ac.id

ABSTRACT

Molecular docking method of several heparin oligomer to FGF2-FGFR1 ligand-receptor complex has been carried out. The receptor have important role to produce signal transduction on anticancer biological cascade. Docking heparin 2-12 saccharides with ^{2}S$_{0}$ iduronic conformation and 2S and 2SNS sulfation pattern on FGF2-FGFR1 ligand-receptor terner complex was carried out using Autodock 4.2 with default Force Field. Docking molecule pose resulted were refined by optimization on YASARA by NOVA AMBER Force Field. The deviations in atomic position of ligands to referred native ligand were determined by RMSD value. The lowest interaction energy score for heparin docking is heparin 2SNS 8 saccharides by -25.01 (kcal/mol). Interactions of heparin take place to Lys, Asn, Gln, Arg amino acids of ligand-receptor complex. The refinement interaction energy of heparin 2SNS 8 saccharides calculated by Yasara is -155.5 kcal/mol. RMSD value for the optimazed structure 2SNS 8 saccharides is 1.497471 Å.

Grand Canonical Monte Carlo Simulation of Hydrogen Molecules Occupancy inside Zeolitic Ice

Muhammad Ruslan Novianto, Zubaidah Ningsih, Lukman Hakim[*]

Dept. of Chemistry, Brawijaya University, Malang

[*]Corresponding email: lukman.chemist@ub.ac.id

ABSTRACT

Hydrogen is a renewable clean fuel that can ease our dependence on fossil energy. One of the challenges in implementing hydrogen-based energy distribution system is the need for efficient and safe hydrogen storage materials. Hydrogen storage using crystalline water is attractive because of the simplicity in composition and the peculiar polymorphs. Water crystal and zeolite share a common aspect in tetrahedral topology. Some ice structures are isomorphic with zeolite structures that have low density whose empty space can be occupied by a large amount of hydrogen molecules. In this work, 243 zeolite structures are adopted into ice structures. The hydrogen occupancies inside each of those structures are investigated using the Grand Canonical Monte Carlo simulation method. Some zeolitic ice structures is found to be mechanically unstable due to the unfavorable configuration of hydrogen bonds. The simulation also shows that the hydrogen storage capacity of zeolitic ice is generally higher than the usual ice storage capacity. From the simulation results, ice RWY has the highest occupancy with a ratio of hydrogen to water is 3.8. This work serves as an initial screening process to the potential of zeolitic ice as a hydrogen storage material.

Free Energy Analysis on Insulin Aggregation Using Energy Representative Method and Molecular Dynamics Simulation

Ellya Indahyanti, Lukman Hakim[*], Diah Mardiana, Ani Mulyasuryani

Dept. of Chemistry, Brawijaya University, Malang

[*]Corresponding email: lukman.chemist@ub.ac.id

ABSTRACT

Insulin has an important role in synthesizing glycogen from glucose. In carrying out the duty in the body, insulin action is influenced by aqueous solvents called the hydrophobic effect. The presence of water solvent affect processes such as improper protein folding, stability and dynamics. One result of these various processes is the existence of aggregation. Amyloid formation and aggregation is the main cause of metabolic and neurodegenerative diseases, such as Parkinson's disease, Alzheimer's disease, and Huntington's disease. In this study, the prevention of aggregation can be done through the addition of urea as co-solvent. The research was carried out using Molecular Dynamics simulation. The energy of aggregation of peptides associated with the presence of solvent can be calculated. Solvation free energy for peptides or their aggregates in solvent are calculated when free energy disturbances or thermodynamic interaction methods are used in molecular simulations. Furthermore, the energy representation method was chosen for free energy analysis.

SYMPOSIUM

Macromolecules and Polymers (POL)

Thermal Analysis of Liquid Crystal Polymer of Mesogen Reactive 82 With Variations of Weight Percentage of Methyl Metacrylate

Afrizal[1], Yusmaniar[1], Maria Paristiowati[1], Darsef[1], Bryan Valentino[1], Umar Kalmar Nizar[2]

[1] *Dept. of Chemistry, Universitas Negeri Jakarta, Jakarta*
[2] *Dept. of Chemistry, Universitas Negeri Padang, Sumatera Barat*

*Corresponding email: afrizal@unj.ac.id

ABSTRACT

Liquid crystal polymer (LCP) Mesogen reactive 82-Polymethyl metacrylate has been successfully synthesized by UV curing method. This research was conducted by varying the weight percent of PMMA, at 0%, 5%, 10%, 20%, and 30% towards reactive mesogen RM82 30%. Thermal analysis using Differential Scanning Calorymeter instrument showed diffractogram that peak of endothermic and exothermic. Every increase weight percent of PMMA causes a shift in the peak towards a lower temperature which will affect the melting and crystallization process quickly. Characterized by microscopy showed the surface-shape transformation from the blade-like fibrous crystal belonging to RM82, to fiber crystals with spheres at the ends with the incorporation of 5% PMMA, and into crystal chunks form by the additional of 30% PMMA. Therefore analysis using X Ray Diffraction showed some sharp peaks at 2θ around 10°, 20°, and 21°. This result indicated that all the formed samples had a crystalline phase and would experience an intensity decreasing with increasing weight percent of PMMA.

Synthesis of Polyvinyl Alcohol-Chitosan Biodegradable Films with Nanocellulose from Coconut Fibers (Cocos Nucifera)

Yusmaniar[*1], Egie Julio[*1], Arif Rahman[*1], Afrizal[*1], Maria Paristiwati [1*]and Renny Juniar[1*]

[1]Dept. of Chemistry. Universitas Negeri Jakarta

[*]Corresponding email: yusmaniar@unj.ac.id

ABSTRACT

In this research, polyvinyl alcohol (PVA) – chitosan biodegradable films were made with nanocellulose from coconut fibers. The process began by separating lignin and hemicellulose through delignification and bleaching, followed by the hydrolysis of cellulose to produce nanocellulose. Furthermore, the polyvinyl alcohol films were mixed with chitosan in certain compositions and added to the nanocellulose in a particular concentration. The results showed that nanocellulose increased the tensile strength of PVA-chitosan biodegradable films with optimal efficiency at 1% concentration based on the total mass with a strength of 35.78 MPa. Additionally, it also increased the degradation of the biodegradable films with optimal conditions at the addition of 10% nanocellulose with a mass loss percentage of 17.07%.

Molecularly Imprinted Polymer (MIP) Chitosan-Based in The Development of Electrochemical Sensor for Caffeine Detection

Ani Mulyasuryani [*1], Hermin Sulystiarti[1], Akhmad Sabarudin[1]

[1] *Dept. of Chemistry, Brawijaya University, Malang*

[*]Corresponding email: mulyasuryani@ub.ac.id

ABSTRACT

Molecularly Imprinted Polymers (MIPs) are synthetic receptors for targeted molecules, they can be applied to the development of molecular sensors. In this application, the MIP is combined with a reading system, either electrically, electrochemically, or optically. Research has been carried out on the effect of caffeine concentration in MIP and type of electrolyte on sensor sensitivity. MIP is made from chitosan, Fe_3O_4 nanoparticles, STPP (sodium tripolyphosphate) as crosslinker, and caffeine as template. The MIP was coated on a glassy carbon (GCE) electrode and heated for 1 hour at 500C. GCE was washed with ethanol for 15 minutes and heated for 15 minutes at 500C. Caffeine in the MIP was removed by cyclic voltammetry (CV) technique. The performance of the sensor was evaluated at eleven concentrations of caffeine solution in the concentration range of 0.5–10 M in 0.1 M H_2SO_4. The optimum caffeine concentration in the MIP is 2% and the optimum type of supporting electrolyte is 0.1 M H_2SO_4. The results showed that the caffeine concentration in MIP and the type of supporting electrolyte influence to the sensitivity of the sensor. The increase in caffeine concentration in MIP is inversely proportional to the sensitivity of the sensor.

SYMPOSIUM

Chemistry Education (EDU)

ChemDuino-Calorimetry to determine the Enthalpy Change of Neutralization of an Acid−Base Reaction: Making a familiar experiment "greener"

N Krisnu Prabowo[1], M Paristiowati[*2], Irwanto[3], Afrizal[4], Yusmaniar[5]

Department of Chemistry Education, Faculty of Mathematics and Natural Science, Universitas Negeri Jakarta, Jakarta, Indonesia

[*]Corresponding email: maria.paristiowati@unj.ac.id

ABSTRACT

The implementation of green chemistry in secondary education aspires to train students and increase their awareness of reducing the chemical usage, and minimize waste produced from experimental activities. However, in a common thermochemistry experiment, a large volume and relatively high concentration of chemicals are often used to get a significant temperature change using an analogue thermometer. A 'greener' experimental protocol is developed as an alternative using modern microcontroller boards, ChemDuino. The aim of this research is to develop a low-cost and pocket-sized prototype for measuring temperature of solutions using Arduino Uno R3 DIP and DS18B20 sensor based on green chemistry and DIY (do-it –yourself) methods. The construction of ChemDuino for temperature sensing is made in the simplest manner for individuals with little knowledge of electronics. The details of all components are stipulated in this paper. This research was conducted in three phases, which includes preliminary, prototype development, and assessment phase. The device is used to determine the enthalpy change of neutralization (ΔH) of NaOH and HCl solution. The enthalpy change of neutralization, kJ mol^{-1} at 25.0 $^{\circ}$C from literature is -57.13 kJ mol^{-1}, whereas the enthalpy change of neutralization, kJ mol^{-1} at 25.0 $^{\circ}$C from the experiment using ChemDuino-Calorimetry is -55.16 $\pm$ 5.2 kJ mol^{-1} (average of seven determinations and estimated standard deviation). The device has successfully measured the temperature change of the reaction at a relatively lower concentration. ChemDuino-Calorimetry has a great potential, because of its reliability and accuracy in measurements, inexpensive setup, and interconnectivity.

INTEGRATION OF TECHNOLOGY IN PROBLEM-BASED LEARNING TO IMPROVE STUDENTS' COMPUTATIONAL THINKING: IMPLEMENTATION ON POLYMER TOPICS

Nurasiah[*1], M paristiowati [2], Erdawati [3] , Afrizal [4]

[1] *Dept. Chemistry Education, Faculty of Mathematics and Natural Science, Universitas Negeri Jakarta, Jakarta, Indonesia*

[*]Corresponding email: nurasiah057201@gmail.com

ABSTRACT

Abstract. This research is motivated by the importance of developing computational thinking skills for students in facing the challenges of the 21st century. Computational thinking is described as a thinking process in formulating problems and solving problems computationally through computers, humans or machines. Its skills can be measured during the learning process of students with the approach of basic computational thinking strategies as follows: Are students able to decompose complex problems into simpler problems? (Decomposition), can students create problem patterns? (Pattern recognition), are students able to focus on issues that are considered important? (Abstraction), and whether students can solve problems systematically (Algorithm) with SMART (specific, measurable, attainable, relevant, time-based). The research aims to improve students' computational thinking skills through the integration of technology in problem-based learning models on polymer topics. This study uses a quasi-experimental quantitative method with none equivalent control group design. The subjects in this study were students of SMAN 1 South Tangerang City, totaling 66 students of class XII. The results showed that the computational thinking skills of students increased after the implementation of the problem-based learning model integrated with technology. This is indicated by the average N-Gain Score for the experimental class which is 56.65%, which is included in the quite effective category, and based on the independent sample t-test. The Sig value is obtained. (2-tailed) 0.007. This indicates Sig. (2-tailed) <, it can be concluded that there is a significant positive effect of the use of technology integration in the problem-based learning model on polymer topics. Keywords: Computational Thinking, Polymer, Problem-Based Learning, Technology.

INTEGRATION OF DIGITAL MEDIA VARIATIONS WITH FLIPPED CLASSROOM MODELS IN CHEMISTRY LEARNING: An Analysis of Student Activities and Learning Outcomes

Roisyah Fitriani[*1], Nur Stifany Kholbunnisa[1], Maria Paristiowati[1], Yusmaniar[1], Hanhan Dianhar[1], and Setia Budi[1]

[1]*Dept. of Chemistry Education, Faculty of Mathematics and Natural Science, State University of Jakarta*

[*]Corresponding email: roisyahfitriani_1303618027@mhs.unj.ac.id

ABSTRACT

This article focuses on the implementation of the flipped classroom model by integrating various digital media in chemistry learning. The variations of digital media used in this research are YouTube, Miro, Wizer.me, Quizizz, Google Form, and Google Classroom. Activities and student learning outcomes in class XI are the variables analyzed. The research method used is a descriptive qualitative method with data collection techniques through observation sheets, teacher diaries, interviews, reflective journals, student activity questionnaires, and learning outcome's tests. The activity questionnaire in this study used StRIP, which was adapted from DeMonbrun et al. Activity indicators in this study consist of two dimensions, as follows the dimensions of student response to instructions and dimensions of the type of instruction. Student activity data is processed using a Likert scale. To find out the students' understanding, a multiple-choice test was used. The results showed that most of the students gave a good response to the second dimension.The results showed that students' responses to instructions and types of instructions during the learning process developed well. This is in accordance with the results of student questionnaire data, which shows a percentage of >70% in each dimension. Overall learning outcomes have increased. In the cognitive domain, the average learning outcomes are above the Minimum Completeness Criteria (KKM). In the affective domain, it shows that some students have a good attitude of responsibility and discipline, actively express opinions and work together in groups. In the psychomotor domain, students show that they are careful in conducting and compiling practicum reports. The conclusion of this study is that the flipped classroom learning model using various digital learning media can help develop student activities and improve student learning outcomes in class XI in chemistry learning.

SYMPOSIUM

Biophysics and Biochemistry (BIO)

UTILIZATION OF NEERA AS A LOW-COST-MEDIUM ALTERNATIVE FOR PRODUCING BACTERIAL NANO-CELLULOSE USING KOMAGATAEIBACTER XYLINUS

Dara P. Hapsari, Claudia P. Gadizza, Setiyo Gunawan[*]

Dept of Chemical Engineering, Sepuluh Nopember Institute of Technology, Surabaya

[*]Corresponding email: gunawan@chem-eng.its.ac.id

ABSTRACT

Bacterial nano-cellulose (BNC) is a natural polymer with excellent character. Compared to other cellulose obtained from the extraction process of plant cellulose, BNC has very high purity because it does not contain impurities, such as lignin and hemicellulose. That is because BNC production is the process of forming cellulose from monosaccharides with the help of acetic acid bacteria. However, the BNC production process cannot be applied in the industry because the media used for BNC production is quite expensive, causing an increase in production costs. Neera is a product derived from tapping the flower of the Siwalan plant. It has a high sugar content, which is around 10-12%, so it has the potential to be used as an alternative medium for producing BNC. The sugar content in neera needs to be maintained by pasteurization. *Komagataeibacter xylinus* from Indonesia Culture Collection (InaCC) was used as acetic acid bacteria to produce BNC. The aim of this study was to discover the optimum media condition to improve the production yield of BNC using neera as alternative media. Neera doesn't have enough nitrogen, which is an important energy source for *K. xylinus* to live. It has low pH after pasteurization, around 3.6-3.7, which is not an ideal condition for producing BNC. Thus, neera needs additional nutrition from ammonium sulfate and molasses as a source of nitrogen and carbon. NaOH also needed to increase the pH of the medium to help the production of BNC. After adding 0.5 g ammonium sulfate, 1 g molasses, and 10 ml NaOH, *K. xylinus* can produce BNC with a yield of 2,58 g/L.

SYMPOSIUM

Metallic Compounds and Metal Organic Frameworks (MET)

Synthesis of Functional Heteronuclear Complex of Fe(III)-Mn(II)-Tartrate

Yuniar Ponco Prananto[*1], Ade Hanindya Rafika[1], Mohammad Misbah Khunur[1], Rachmat Triandi Tjahjanto, Galuh Wahyu Karti'a[1]

[1] *Department of Chemistry, Brawijaya University, Malang*

[*]Corresponding email: prananto@ub.ac.id

ABSTRACT

Synthesis of functional heteronuclear complexes of Fe(III)-Mn(II)-tartrate is reported here. Effect of Fe(III) salts and reaction temperature in the solvothermal synthesis of the targeted complex is also investigated. $FeCl_3$ and $NH_4Fe(SO_4)_2$ were used as the precursor of Fe(III), which then mixed with solutions of $MnCl_2$ and *L*-tartaric acid with a Fe(III)-Mn(II)-tartrate molar ratio of 2:2:5 in the 50 mL of Teflon-autoclave. A mixture of dimethyl formamide and distilled water (1:3) was used as the solvent. The solvothermal reactions were done at 110 and 130 C, respectively, for 2 hours. Solids which precipitated out from the reaction, were separated, dried in an oven and then characterised by Fourier Transform Infrared (FTIR) spectroscopy and atomic absorption spectrophotometer (AAS). Experimental data shows that all four reactions resulted in identical pale yellow-greenish fine powder which indicates that the Fe(III) precursor and reaction temperature did not affect the synthesised complex. However, the yield were different among those four reactions. FTIR analysis confirm the presence of tartrate ligand based on specific absorptions, namely a broad band around 3400 (O–H) cm^{-1}, sharp peak around 1650 (O–C=O) cm^{-1}, twin sharp peaks between 1400-1100 (C–OH) cm^{-1}. Moreover, AAS confirm the presence of both Fe and Mn in all samples in a considerably significant amount. Based on this two initial characterisation, it is highly expected that the fine powders were Fe(III)-Mn(II)-tartrate complex. To fully characterise the product and investigate the effect of Fe(III) precursor and reaction temperature on the properties of the complex, further characterisation by powder XRD, SEM, and melting point test are done and still ongoing.

Entonox Scavenging Reduction Through Gaseous Adsorption in Zirconium based Metal Organic Frameworks

Rama Oktavian[*12], Robert Musimbago[1], Mattie Tawana[1], Peyman Z. Moghadam[*1]

[1] *Department of Chemical and Biological Engineering, The University of Sheffield, UK*
[2] *Department of Chemical Engineering, Brawijaya University.*

[*]Corresponding email: roktavian1@sheffield.ac.uk p.moghadam@sheffield.ac.uk

ABSTRACT

Nitrous oxide has been used as laughing gas, an anaesthetic in surgery, dentistry, and maternity. Laughing gas has been dispensed as Entonox® a blend between nitrous oxide gas and oxygen gas in a 1:1 ratio. Subsequently, chronic occupational exposure to nitrous oxide at scavenging levels above 100 p.p.m has been linked to B12 anaemias, fetotoxicity and miscarriages. Therefore, Control of Substances Hazardous to Health (COSHH) standards have limited the 8-hour weighted average exposure to 100 p.p.m in all work settings. However, many health facilities do not have the ventilation standard needed to keep exposure below this limit and health workers are always exposed to scavenging levels above this limit. And there has not yet been an anaesthetic gas alternative to nitrous oxide. There is therefore an urgent need to reduce Entonox scavenging in health facilities. A novel adsorption methods using Metal Organic Frameworks (MOFs) could be employed in Etonox scavenging reduction process. We investigated the adsorption capabilities of materials belonging to a class of MOFs, Zirconium oxide MOFs (Zr-MOFs) by High Throughput Screening (HTS) utilizing the Grand Canonical Monte Carlo (GCMC). We then simulated the adsorption of N2O in 40 Zirconium oxide MOFs, which we screened and identified top-performing MOF candidate (CSD reference code: QURNOI) to have the highest N2O capture of 9.32mmol/g at 298K and 1 bar. Our molecular simulation revealed that binding of N2O to adsorbent was majorly via electrostatic interaction and high pore volumes did not necessary lead to elevated adsorption capacities in Zr-MOFs.

POSTER ABSTRACTS